```
* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1            Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2            "Ask CAS" for self-help around the clock
 NEWS  3  SEP 09    CA/CAplus records now contain indexing from 1907 to the
                    present
 NEWS  4  DEC 08    INPADOC: Legal Status data reloaded
 NEWS  5  SEP 29    DISSABS now available on STN
 NEWS  6  OCT 10    PCTFULL: Two new display fields added
 NEWS  7  OCT 21    BIOSIS file reloaded and enhanced
 NEWS  8  OCT 28    BIOSIS file segment of TOXCENTER reloaded and enhanced
 NEWS  9  NOV 24    MSDS-CCOHS file reloaded
 NEWS 10  DEC 08    CABA reloaded with left truncation
 NEWS 11  DEC 08    IMS file names changed
 NEWS 12  DEC 09    Experimental property data collected by CAS now available
                    in REGISTRY
 NEWS 13  DEC 09    STN Entry Date available for display in REGISTRY and CA/CAplus
 NEWS 14  DEC 17    DGENE: Two new display fields added
 NEWS 15  DEC 18    BIOTECHNO no longer updated
 NEWS 16  DEC 19    CROPU no longer updated; subscriber discount no longer
                    available
 NEWS 17  DEC 22    Additional INPI reactions and pre-1907 documents added to CAS
                    databases
 NEWS 18  DEC 22    IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
 NEWS 19  DEC 22    ABI-INFORM now available on STN
 NEWS 20  JAN 27    Source of Registration (SR) information in REGISTRY updated
                    and searchable
 NEWS 21  JAN 27    A new search aid, the Company Name Thesaurus, available in
                    CA/CAplus
 NEWS 22  FEB 05    German (DE) application and patent publication number format
                    changes
 NEWS 23  MAR 03    MEDLINE and LMEDLINE reloaded
 NEWS 24  MAR 03    MEDLINE file segment of TOXCENTER reloaded
 NEWS 25  MAR 03    FRANCEPAT now available on STN

 NEWS EXPRESS  MARCH 5 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 20:35:55 ON 14 MAR 2004

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
```

FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 20:36:00 ON 14 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 MAR 2004 HIGHEST RN 662722-88-5
DICTIONARY FILE UPDATES: 12 MAR 2004 HIGHEST RN 662722-88-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

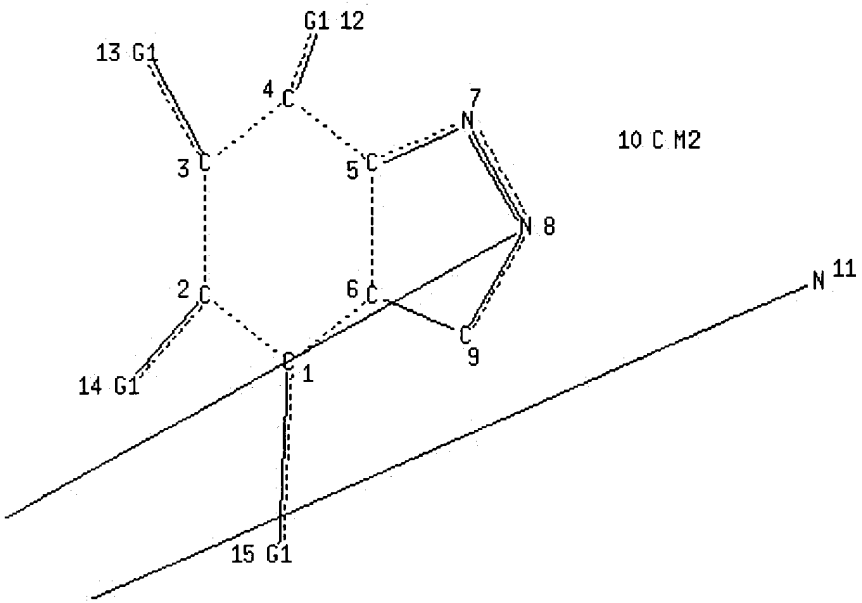
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1 STRUCTURE UPLOADED

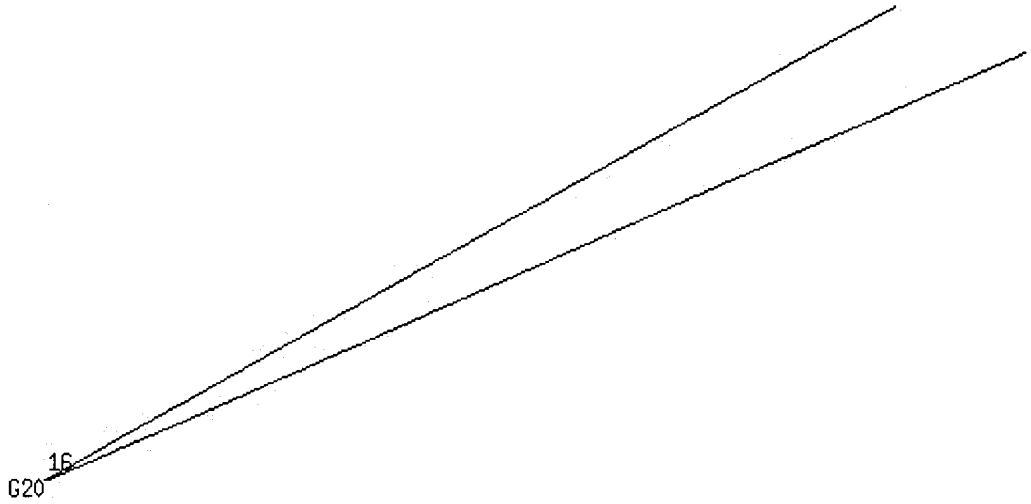
=> d l1
L1 HAS NO ANSWERS
L1 STR

H 17 X 18

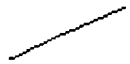
Page 1-A



Page 1-B



Page 2-A

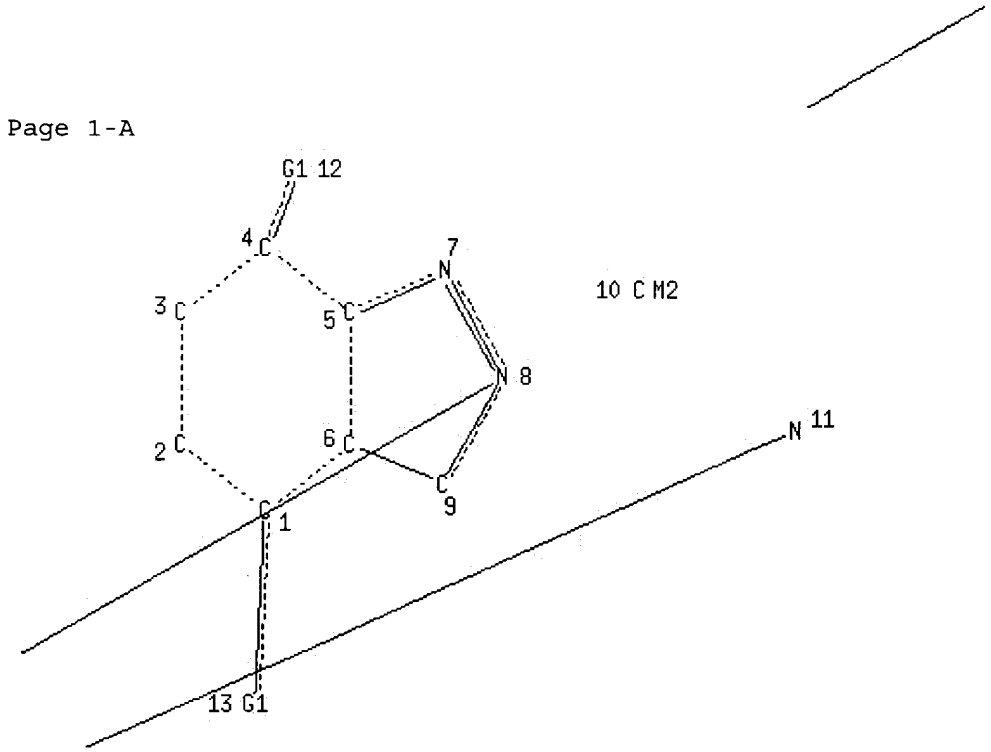


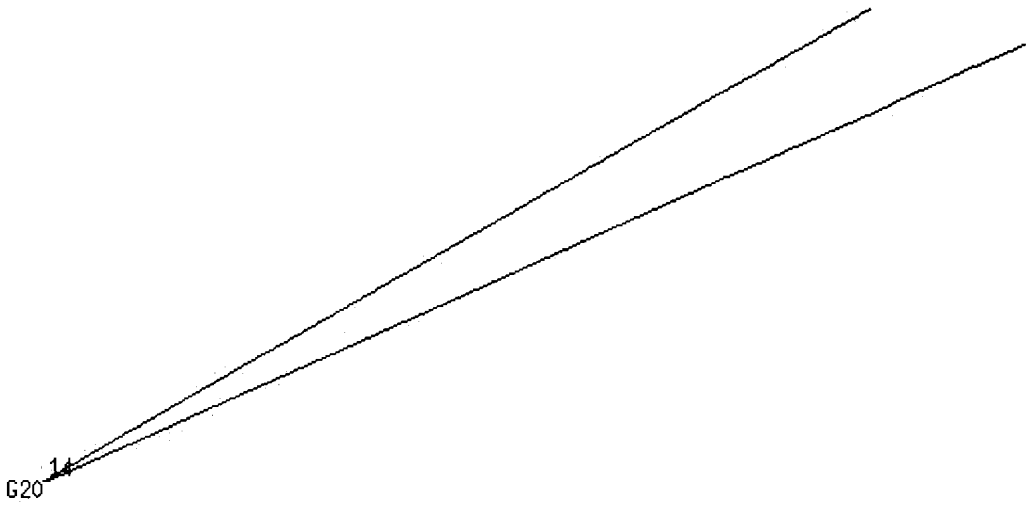
Page 2-B

```
VAR G1=17/18
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:
HCOUNT   IS M2     AT  10
NSPEC    IS R      AT   1
NSPEC    IS R      AT   2
NSPEC    IS R      AT   3
NSPEC    IS R      AT   4
NSPEC    IS R      AT   5
NSPEC    IS R      AT   6
NSPEC    IS R      AT   7
NSPEC    IS R      AT   8
NSPEC    IS R      AT   9
NSPEC    IS C      AT  10
NSPEC    IS R      AT  11
NSPEC    IS C      AT  12
```

```
NSPEC   IS C      AT  13
NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
NSPEC   IS C      AT  16
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  10 17 18
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  18

STEREO ATTRIBUTES: NONE


=> s l1
SAMPLE SEARCH INITIATED 20:39:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    209 TO ITERATE

100.0% PROCESSED     209 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         3313 TO     5047
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:39:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   4165 TO ITERATE

100.0% PROCESSED    4165 ITERATIONS                               0 ANSWERS
SEARCH TIME: 00.00.01

L3            0 SEA SSS FUL L1

=>
L4      STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4              STR
```

H 15 X 16





Page 2-A

Page 2-B
VAR G1=15/16
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:
HCOUNT IS M2 AT 10
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
NSPEC IS C AT 10
NSPEC IS R AT 11
NSPEC IS C AT 12
NSPEC IS C AT 13
NSPEC IS C AT 14
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 10 15 16
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 16

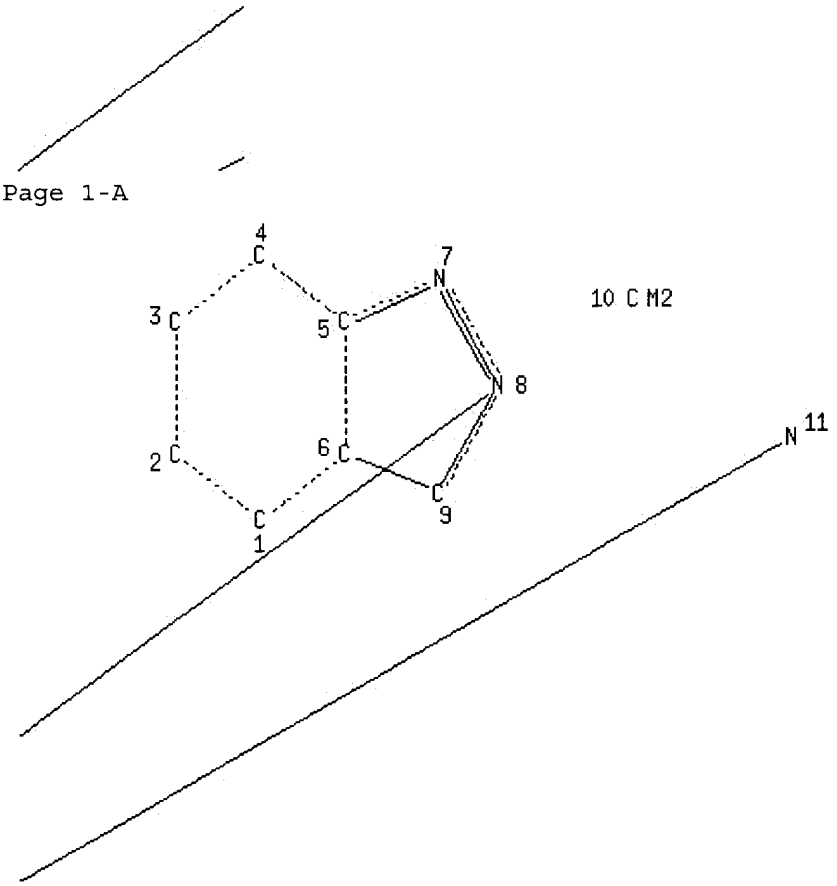
STEREO ATTRIBUTES: NONE

=> **s 14**
SAMPLE SEARCH INITIATED 20:41:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 209 TO ITERATE

100.0% PROCESSED 209 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

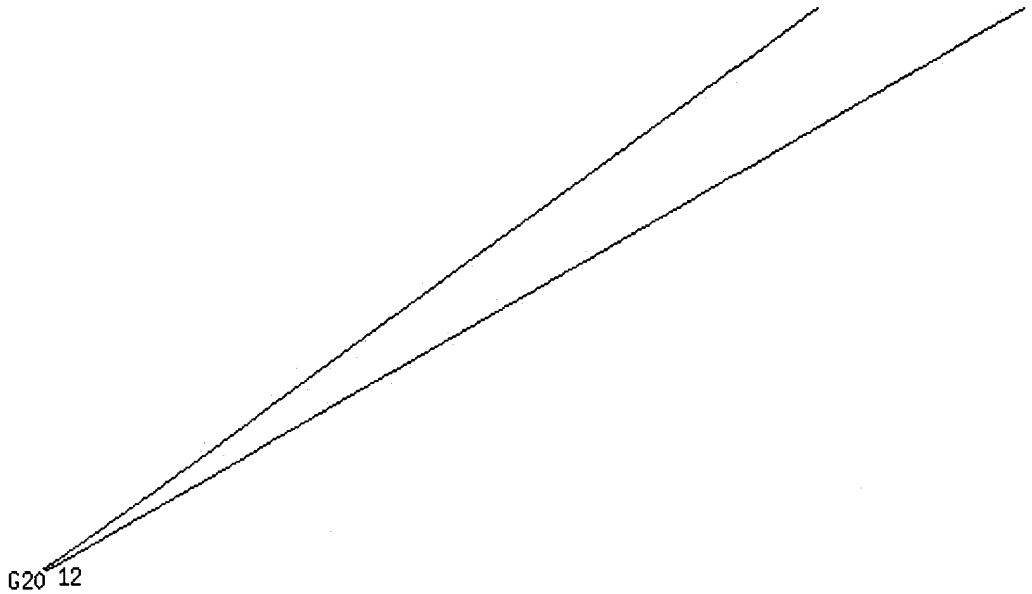
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

```
PROJECTED ITERATIONS:          3313 TO     5047
PROJECTED ANSWERS:                0 TO        0

L5             0 SEA SSS SAM L4

=> s l4 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:41:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   4165 TO ITERATE

100.0% PROCESSED    4165 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

L6             0 SEA SSS FUL L4

=>
L7      STRUCTURE UPLOADED

=> d l7
L7 HAS NO ANSWERS
L7                STR
```



Page 1-A

Page 1-B



Page 2-A

Page 2-B
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:
HCOUNT IS M2 AT 10
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
NSPEC IS C AT 10
NSPEC IS R AT 11
NSPEC IS C AT 12
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 10
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 12

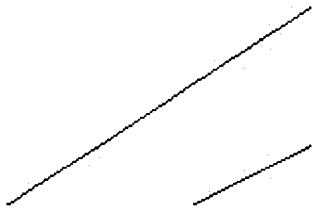
STEREO ATTRIBUTES: NONE

=> s l7
SAMPLE SEARCH INITIATED 20:42:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 209 TO ITERATE

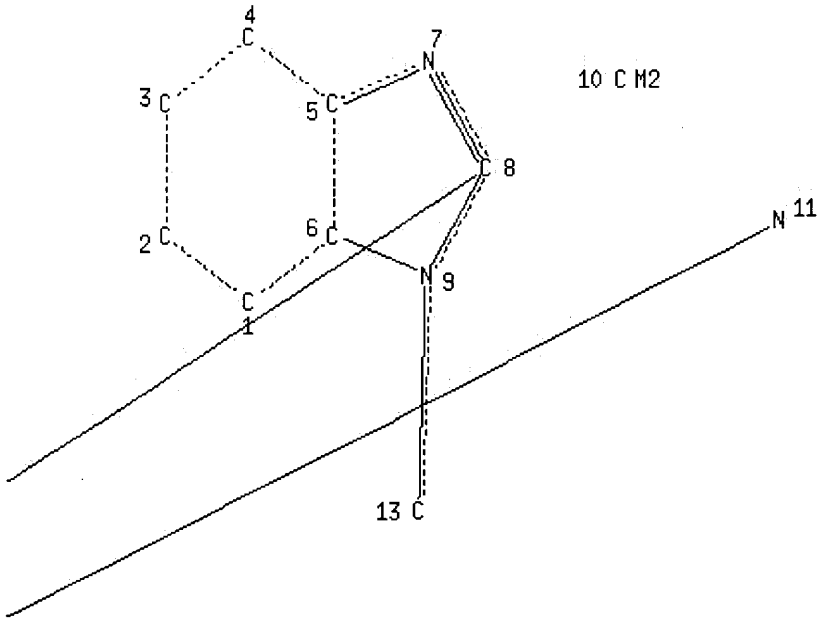
100.0% PROCESSED 209 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3313 TO 5047

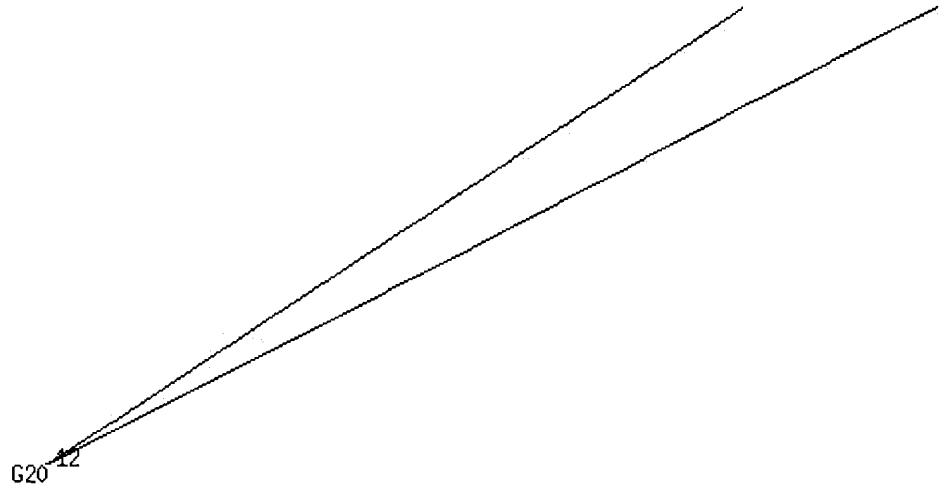
```
PROJECTED ANSWERS:                0 TO        0

L8             0 SEA SSS SAM L7

=> s l7 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:42:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   4165 TO ITERATE

100.0% PROCESSED    4165 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

L9             0 SEA SSS FUL L7

=>
L10      STRUCTURE UPLOADED

=> d l10
L10 HAS NO ANSWERS
L10               STR
```



Page 1-A



Page 1-B

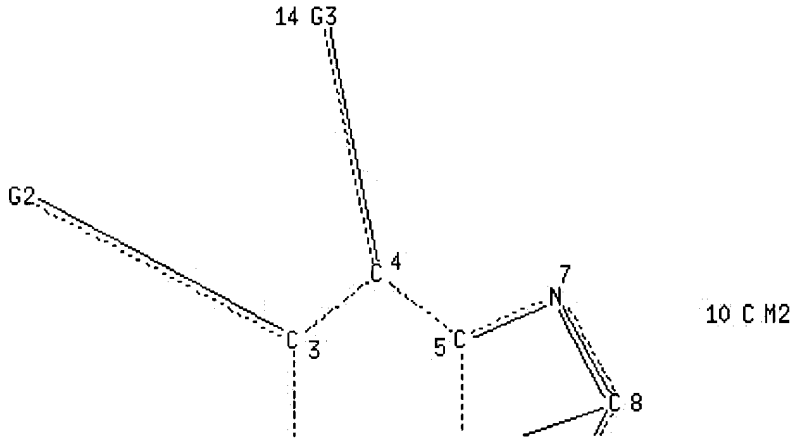



```
Page 2-A
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:
HCOUNT   IS M2      AT  10
NSPEC    IS R       AT   1
NSPEC    IS R       AT   2
NSPEC    IS R       AT   3
NSPEC    IS R       AT   4
NSPEC    IS R       AT   5
NSPEC    IS R       AT   6
NSPEC    IS R       AT   7
NSPEC    IS R       AT   8
NSPEC    IS R       AT   9
NSPEC    IS C       AT  10
NSPEC    IS R       AT  11
NSPEC    IS C       AT  12
NSPEC    IS C       AT  13
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS   AT  10 13
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE


=> s l10
SAMPLE SEARCH INITIATED 20:44:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    483 TO ITERATE

100.0% PROCESSED     483 ITERATIONS                          50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         8342 TO    10978
PROJECTED ANSWERS:            1674 TO     2966

L11          50 SEA SSS SAM L10
```

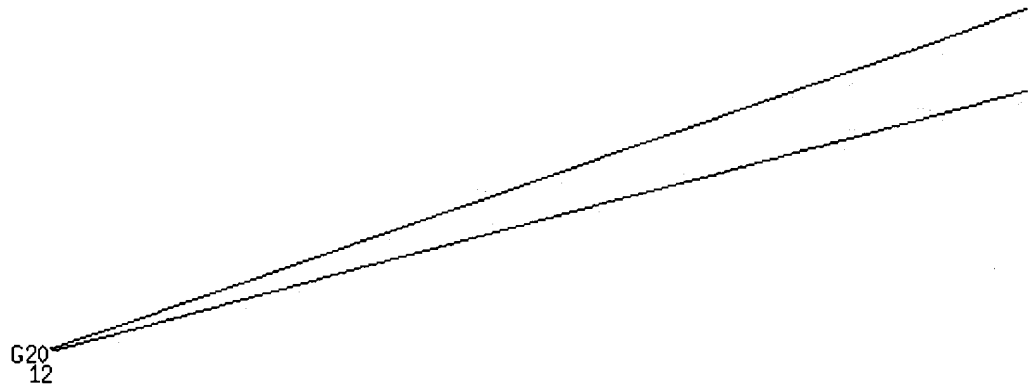
```
=>
L12      STRUCTURE UPLOADED

=> d l12
L12 HAS NO ANSWERS
L12                STR
 H 25 Ak 26

 X 23 H 24

 H 20 X 21 Ak 22
```

16

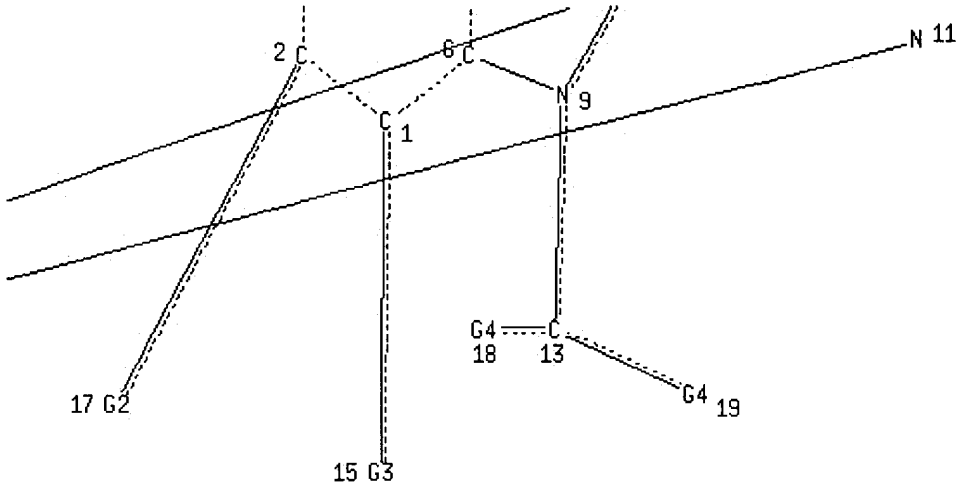
Page 1-A



Page 1-B



Page 2-A



Page 2-B
VAR G2=20/21/22
VAR G3=23/24
VAR G4=25/26
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:
HCOUNT IS M2 AT 10
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
NSPEC IS C AT 10
NSPEC IS R AT 11
NSPEC IS C AT 12
NSPEC IS C AT 13
NSPEC IS C AT 14
NSPEC IS C AT 15
NSPEC IS C AT 16
NSPEC IS C AT 17
NSPEC IS C AT 18
NSPEC IS C AT 19
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 10 13 20 21 22 23 24 25 26
DEFAULT ECLEVEL IS LIMITED

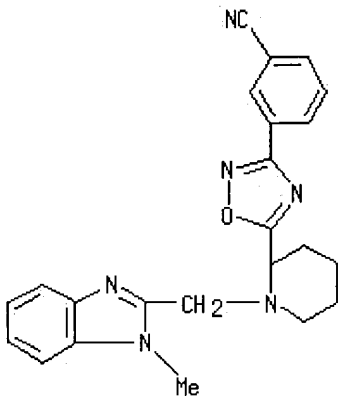
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

=> s l12
SAMPLE SEARCH INITIATED 20:47:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 483 TO ITERATE

100.0% PROCESSED 483 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

```
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          8342 TO    10978
PROJECTED ANSWERS:             1503 TO     2737

L13          50 SEA SSS SAM L12

=> s l12 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:47:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  10274 TO ITERATE

100.0% PROCESSED   10274 ITERATIONS                          2143 ANSWERS
SEARCH TIME: 00.00.01

L14        2143 SEA SSS FUL L12

=> d l14

L14  ANSWER 1 OF 2143  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   661458-71-5  REGISTRY
CN   INDEX NAME NOT YET ASSIGNED
FS   3D CONCORD
MF   C23 H22 N6 O
SR   CA
LC   STN Files:   CAPLUS
```




```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

               1 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=> d his

     (FILE 'HOME' ENTERED AT 20:35:55 ON 14 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 20:36:00 ON 14 MAR 2004
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           0 S L1 FULL
L4             STRUCTURE UPLOADED
```

```
L5              0 S L4
L6              0 S L4 FULL
L7                STRUCTURE UPLOADED
L8              0 S L7
L9              0 S L7 FULL
L10               STRUCTURE UPLOADED
L11            50 S L10
L12               STRUCTURE UPLOADED
L13            50 S L12
L14          2143 S L12 FULL

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   630.17     630.38

FILE 'HCAPLUS' ENTERED AT 20:48:14 ON 14 MAR 2004
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FILE COVERS 1907 - 14 Mar 2004  VOL 140 ISS 12
FILE LAST UPDATED: 12 Mar 2004  (20040312/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l14
L15          259 L14

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     2.36     632.74

FILE 'REGISTRY' ENTERED AT 20:48:25 ON 14 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   12 MAR 2004  HIGHEST RN 662722-88-5
DICTIONARY FILE UPDATES:  12 MAR 2004  HIGHEST RN 662722-88-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004
```

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L16 STRUCTURE UPLOADED

=> d l16
L16 HAS NO ANSWERS
L16 STR

C 32 O 33 N 34

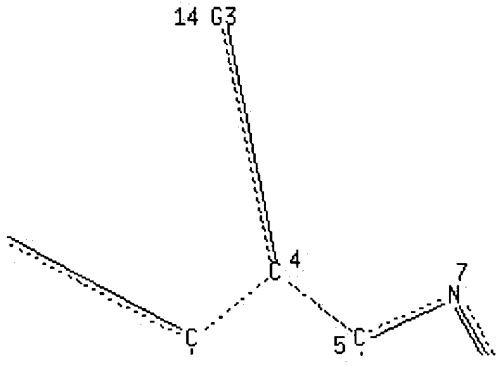
H 30 Ak 31

X 28 H 29

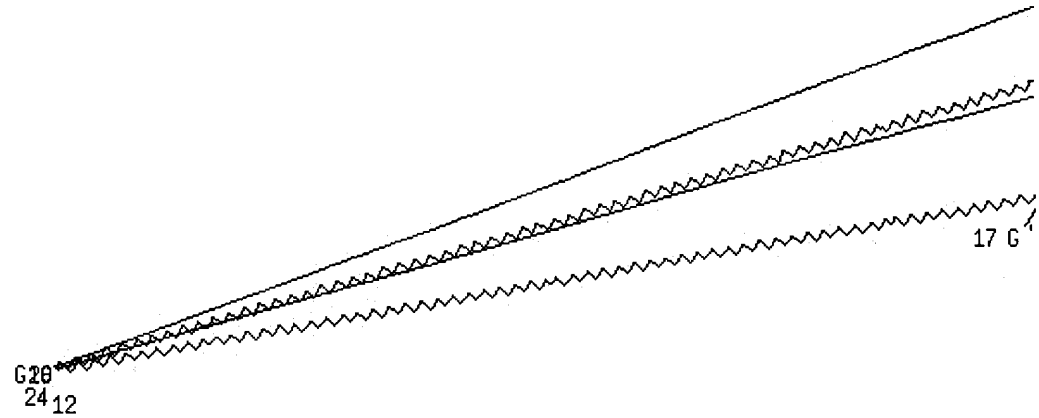
H 25 X 26 Ak 27

16 G2

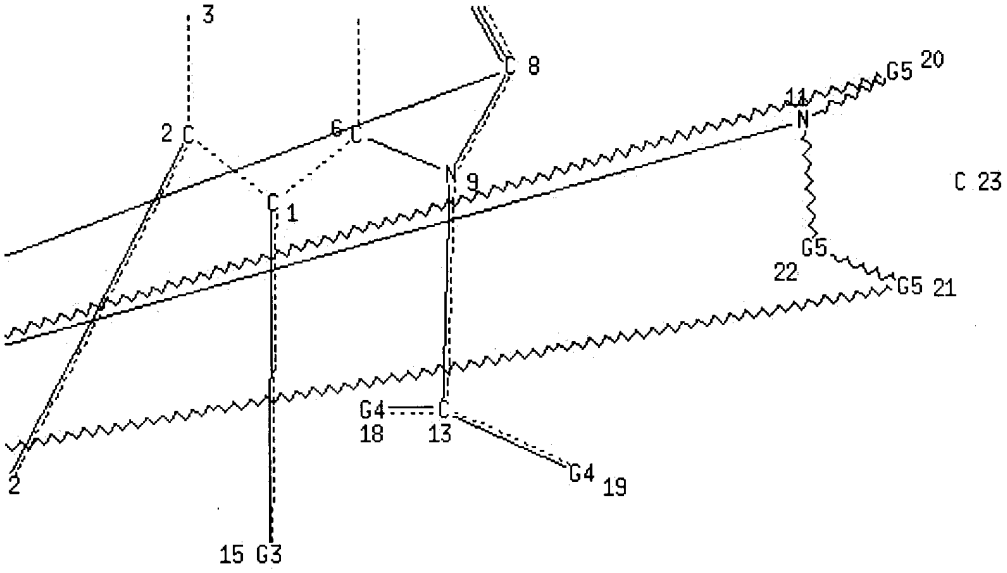
Page 1-A



Page 1-B



Page 2-A



Page 2-B

```
VAR G2=25/26/27
VAR G3=28/29
VAR G4=30/31
VAR G5=32/33/34
REP G19=(1-2) 23-20 23-21
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:
HCOUNT  IS M2     AT  10
NSPEC   IS R      AT   1
NSPEC   IS R      AT   2
NSPEC   IS R      AT   3
NSPEC   IS R      AT   4
NSPEC   IS R      AT   5
NSPEC   IS R      AT   6
NSPEC   IS R      AT   7
NSPEC   IS R      AT   8
NSPEC   IS R      AT   9
NSPEC   IS C      AT  10
NSPEC   IS R      AT  11
NSPEC   IS C      AT  12
NSPEC   IS C      AT  13
NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
NSPEC   IS C      AT  16
```

```
NSPEC   IS C      AT  17
NSPEC   IS C      AT  18
NSPEC   IS C      AT  19
NSPEC   IS R      AT  20
NSPEC   IS R      AT  21
NSPEC   IS R      AT  22
NSPEC   IS R      AT  23
NSPEC   IS R      AT  24
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  10 13 25 26 27 28 29 30 31
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   8
NUMBER OF NODES IS  34

STEREO ATTRIBUTES: NONE


=> s l16
SAMPLE SEARCH INITIATED 20:52:30 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    483 TO ITERATE

100.0% PROCESSED     483 ITERATIONS                          50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         8342 TO    10978
PROJECTED ANSWERS:            1114 TO     2206

L17          50 SEA SSS SAM L16

=> s l16 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:52:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  10274 TO ITERATE

100.0% PROCESSED   10274 ITERATIONS                        1605 ANSWERS
SEARCH TIME: 00.00.02

L18        1605 SEA SSS FUL L16

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              157.94     790.68

FILE 'HCAPLUS' ENTERED AT 20:52:42 ON 14 MAR 2004
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```

FILE COVERS 1907 - 14 Mar 2004 VOL 140 ISS 12
FILE LAST UPDATED: 12 Mar 2004 (20040312/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l18
L19 210 L18

=> s l19 and pd < january 2001
21301832 PD < JANUARY 2001
(PD<20010100)
L20 183 L19 AND PD < JANUARY 2001

=>
L21 STRUCTURE UPLOADED

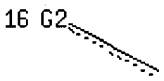
=> d l21
L21 HAS NO ANSWERS
L21 STR

C 35 O 36 N 37

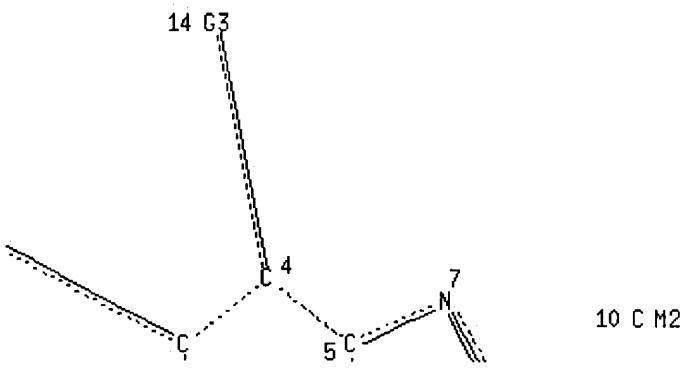
H 33 Ak 34

X 31 H 32

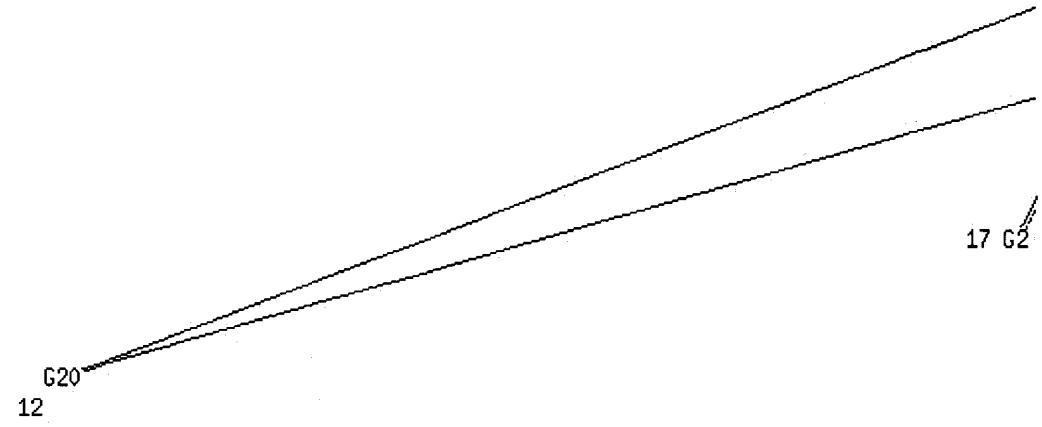
H 28 X 29 Ak 30



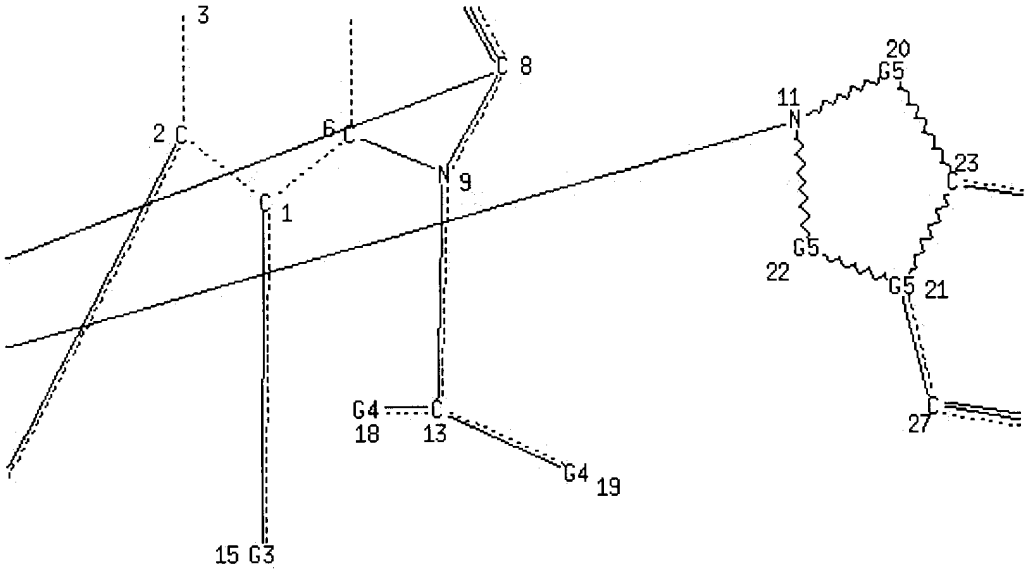
Page 1-A



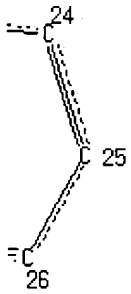
Page 1-B



Page 2-A



Page 2-B



Page 2-C

VAR G2=28/29/30
VAR G3=31/32
VAR G4=33/34
VAR G5=35/36/37
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:
HCOUNT IS M2 AT 10
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4

```
NSPEC   IS R      AT   5
NSPEC   IS R      AT   6
NSPEC   IS R      AT   7
NSPEC   IS R      AT   8
NSPEC   IS R      AT   9
NSPEC   IS C      AT  10
NSPEC   IS R      AT  11
NSPEC   IS C      AT  12
NSPEC   IS C      AT  13
NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
NSPEC   IS C      AT  16
NSPEC   IS C      AT  17
NSPEC   IS C      AT  18
NSPEC   IS C      AT  19
NSPEC   IS R      AT  20
NSPEC   IS R      AT  21
NSPEC   IS R      AT  22
NSPEC   IS R      AT  23
NSPEC   IS R      AT  24
NSPEC   IS R      AT  25
NSPEC   IS R      AT  26
NSPEC   IS R      AT  27
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  10 13 28 29 30 31 32 33 34
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   8
NUMBER OF NODES IS  37

STEREO ATTRIBUTES: NONE


=> s l21
 REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.




SAMPLE SEARCH INITIATED 20:56:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    458 TO ITERATE

100.0% PROCESSED     458 ITERATIONS                              4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         7877 TO    10443
PROJECTED ANSWERS:               4 TO      200

L22           4 SEA SSS SAM L21



L23           3 L22
```

```
=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         2.36     807.62

FILE 'REGISTRY' ENTERED AT 20:56:27 ON 14 MAR 2004
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STRUCTURE FILE UPDATES:   12 MAR 2004  HIGHEST RN 662722-88-5
DICTIONARY FILE UPDATES:  12 MAR 2004  HIGHEST RN 662722-88-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L24      STRUCTURE UPLOADED

=> d l24
L24 HAS NO ANSWERS
L24              STR
 C 35 O 36 N 37


 H 33 Ak 34


 X 31 H 32


 H 28 X 29 Ak 30
```
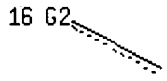
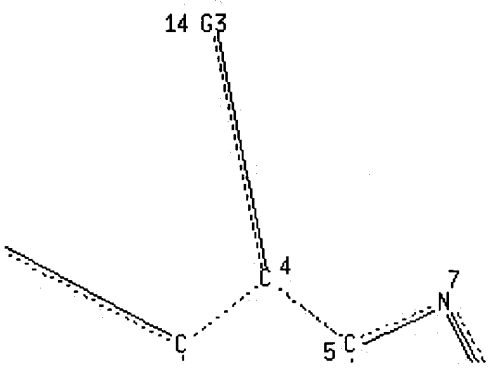
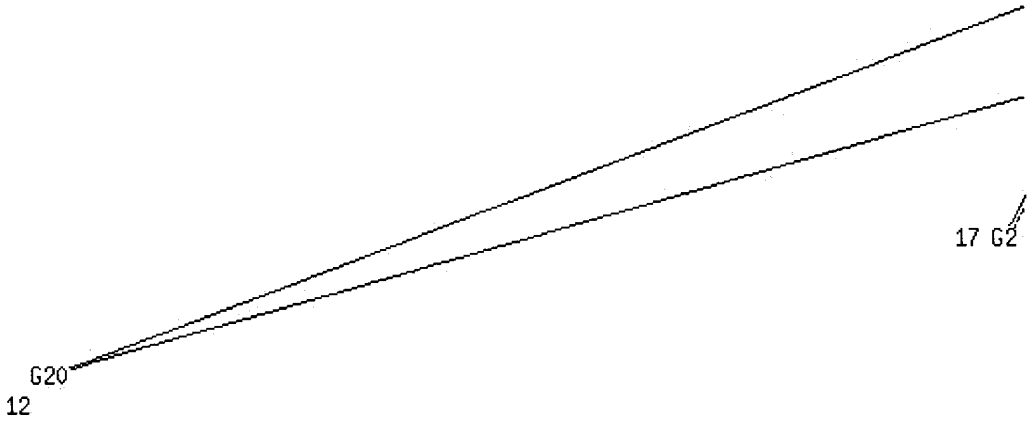



Page 1-A

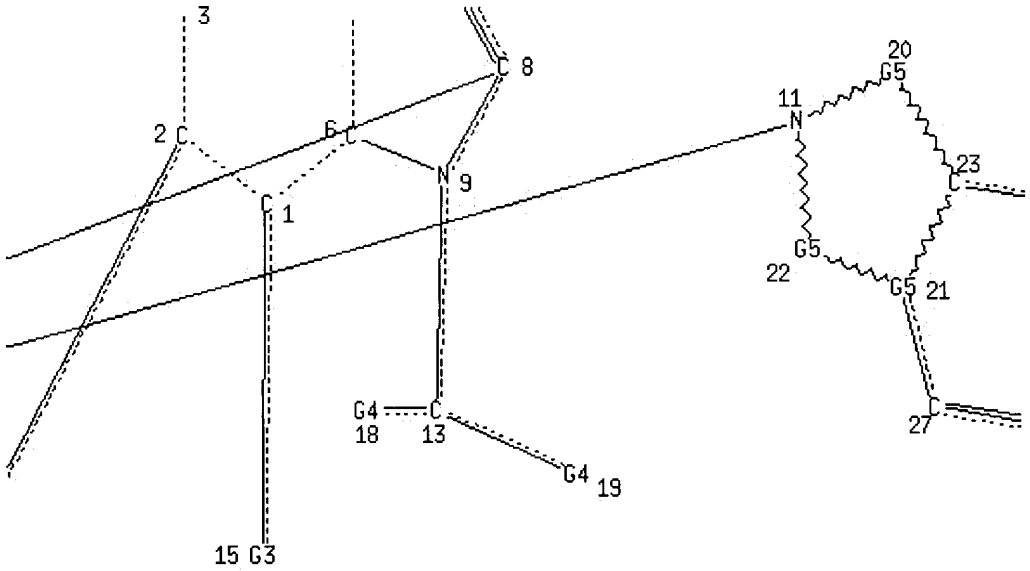


10 C M2

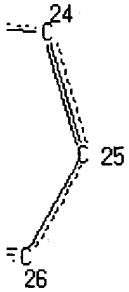
Page 1-B



Page 2-A



Page 2-B



```
Page 2-C
VAR G2=28/29/30
VAR G3=31/32
VAR G4=33/34
VAR G5=35/36/37
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:
HCOUNT  IS M2     AT  10
NSPEC   IS R      AT   1
NSPEC   IS R      AT   2
NSPEC   IS R      AT   3
NSPEC   IS R      AT   4
NSPEC   IS R      AT   5
NSPEC   IS R      AT   6
NSPEC   IS R      AT   7
NSPEC   IS R      AT   8
NSPEC   IS R      AT   9
NSPEC   IS C      AT  10
NSPEC   IS R      AT  11
NSPEC   IS C      AT  12
NSPEC   IS C      AT  13
NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
NSPEC   IS C      AT  16
NSPEC   IS C      AT  17
NSPEC   IS C      AT  18
NSPEC   IS C      AT  19
NSPEC   IS R      AT  20
NSPEC   IS R      AT  21
NSPEC   IS R      AT  22
NSPEC   IS R      AT  23
NSPEC   IS R      AT  24
NSPEC   IS R      AT  25
NSPEC   IS R      AT  26
NSPEC   IS R      AT  27
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  10 13 28 29 30 31 32 33 34
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   8
NUMBER OF NODES IS  37

STEREO ATTRIBUTES: NONE


=> s l24
SAMPLE SEARCH INITIATED 20:56:44 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    458 TO ITERATE

100.0% PROCESSED     458 ITERATIONS                          4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         7877 TO    10443
PROJECTED ANSWERS:               4 TO      200

L25           4 SEA SSS SAM L24
```

```
=> s l24 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:56:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   9691 TO ITERATE

100.0% PROCESSED    9691 ITERATIONS                              98 ANSWERS
SEARCH TIME: 00.00.01

L26           98 SEA SSS FUL L24

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   155.42     963.04

FILE 'HCAPLUS' ENTERED AT 20:56:54 ON 14 MAR 2004
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FILE LAST UPDATED: 12 Mar 2004  (20040312/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l26
L27           13 L26

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     2.36     965.40

FILE 'REGISTRY' ENTERED AT 20:57:08 ON 14 MAR 2004
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STRUCTURE FILE UPDATES:    12 MAR 2004  HIGHEST RN 662722-88-5
DICTIONARY FILE UPDATES:   12 MAR 2004  HIGHEST RN 662722-88-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004
```

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L28 STRUCTURE UPLOADED

=> d 128
L28 HAS NO ANSWERS
L28 STR

C 38 N 39

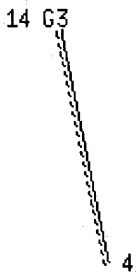
C 35 O 36 N 37

H 33 Ak 34

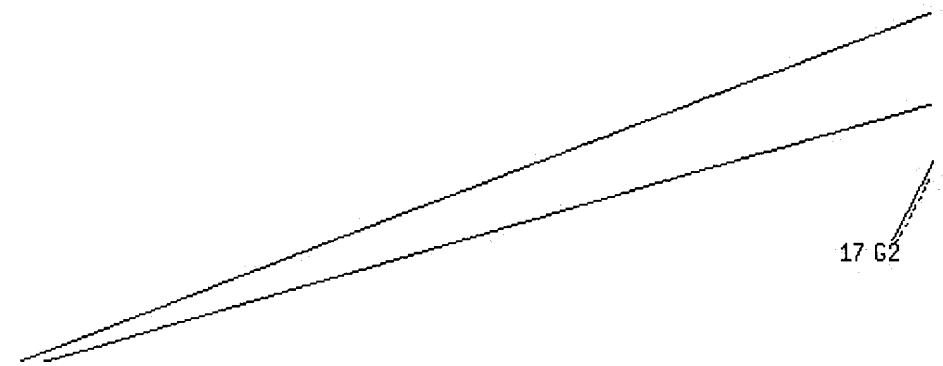
X 31 H 32

H 28 X 29 Ak 30

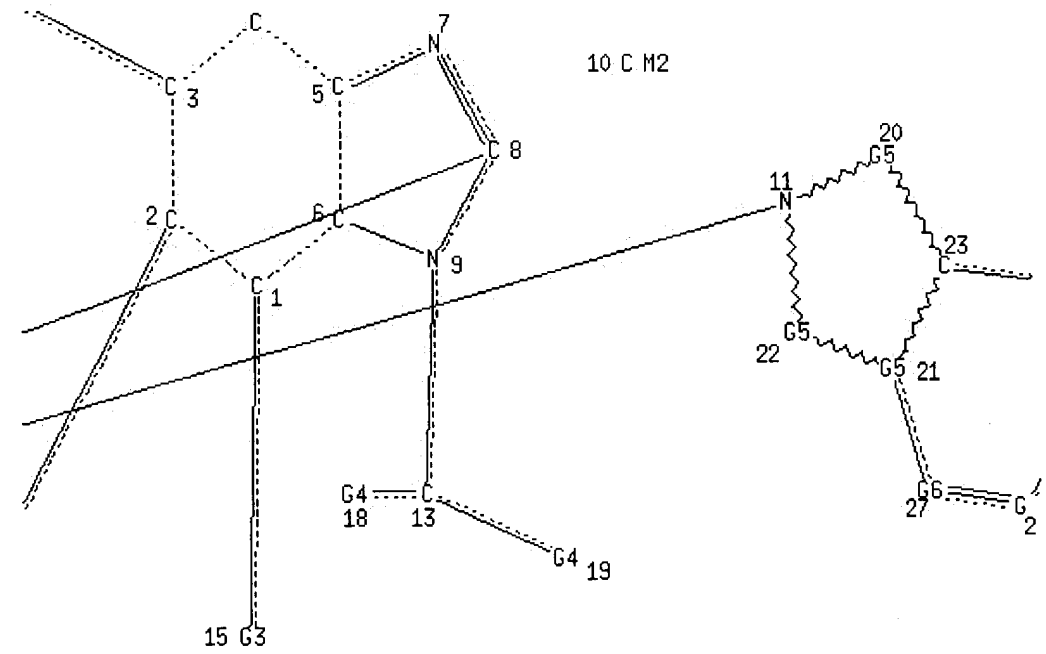
Page 1-A



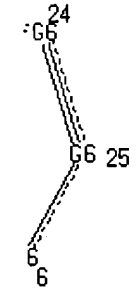
Page 1-B



Page 2-A



Page 2-B



Page 2-C


```
Page 3-A
VAR G2=28/29/30
VAR G3=31/32
VAR G4=33/34
VAR G5=35/36/37
VAR G6=38/39
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:
HCOUNT  IS M2     AT  10
NSPEC   IS R      AT   1
NSPEC   IS R      AT   2
NSPEC   IS R      AT   3
NSPEC   IS R      AT   4
NSPEC   IS R      AT   5
NSPEC   IS R      AT   6
NSPEC   IS R      AT   7
NSPEC   IS R      AT   8
NSPEC   IS R      AT   9
NSPEC   IS C      AT  10
NSPEC   IS R      AT  11
NSPEC   IS C      AT  12
NSPEC   IS C      AT  13
NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
NSPEC   IS C      AT  16
NSPEC   IS C      AT  17
NSPEC   IS C      AT  18
NSPEC   IS C      AT  19
NSPEC   IS R      AT  20
NSPEC   IS R      AT  21
NSPEC   IS R      AT  22
NSPEC   IS R      AT  23
NSPEC   IS R      AT  24
NSPEC   IS R      AT  25
NSPEC   IS R      AT  26
NSPEC   IS R      AT  27
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  10 13 28 29 30 31 32 33 34
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   8
NUMBER OF NODES IS  39

STEREO ATTRIBUTES: NONE


=> s l28
SAMPLE SEARCH INITIATED 20:59:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     483 TO ITERATE

100.0% PROCESSED      483 ITERATIONS                                4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
```

```
PROJECTED ITERATIONS:          8342 TO    10978
PROJECTED ANSWERS:                4 TO      200

L29            4 SEA SSS SAM L28

=> s l29 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:59:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  10268 TO ITERATE

100.0% PROCESSED   10268 ITERATIONS                          98 ANSWERS
SEARCH TIME: 00.00.01

L30            98 SEA SSS FUL L28

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             156.68    1122.08

FILE 'HCAPLUS' ENTERED AT 20:59:15 ON 14 MAR 2004
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FILE COVERS 1907 - 14 Mar 2004  VOL 140 ISS 12
FILE LAST UPDATED: 12 Mar 2004  (20040312/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l30
L31            13 L30

=> file reg
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               2.36    1124.44

FILE 'REGISTRY' ENTERED AT 20:59:25 ON 14 MAR 2004
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```

STRUCTURE FILE UPDATES: 12 MAR 2004 HIGHEST RN 662722-88-5
DICTIONARY FILE UPDATES: 12 MAR 2004 HIGHEST RN 662722-88-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L32 STRUCTURE UPLOADED

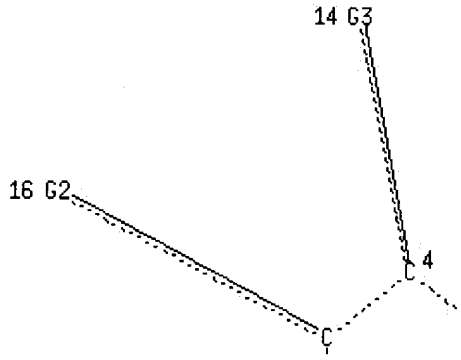
=> d l32
L32 HAS NO ANSWERS
L32 STR

0 33 S 34

H 31 Ak 32

X 29 H 30

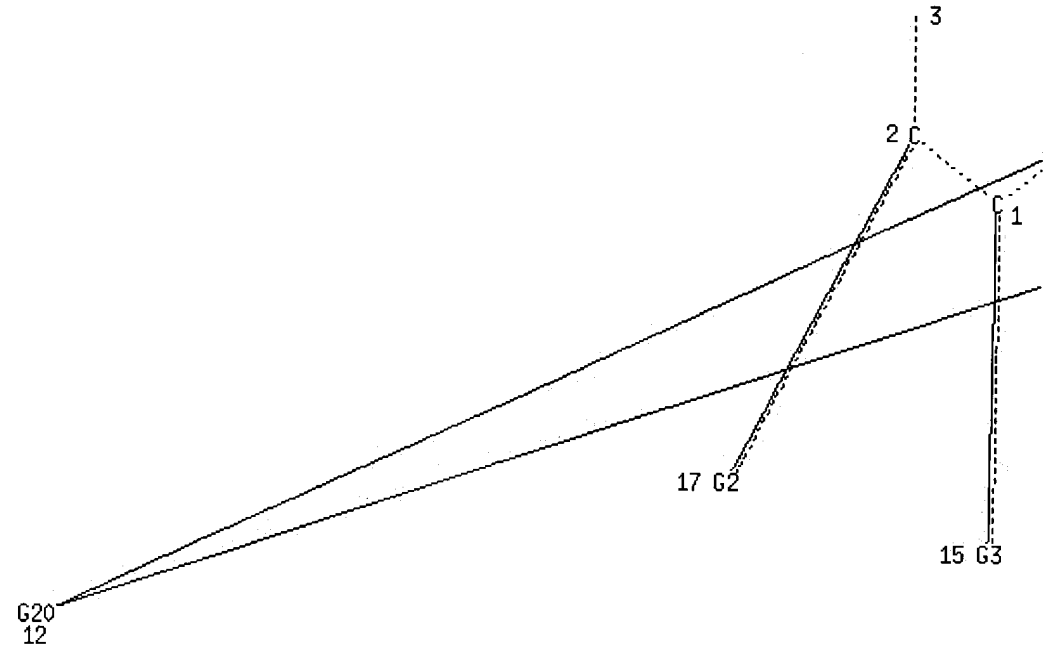
H 26 X 27 Ak 28



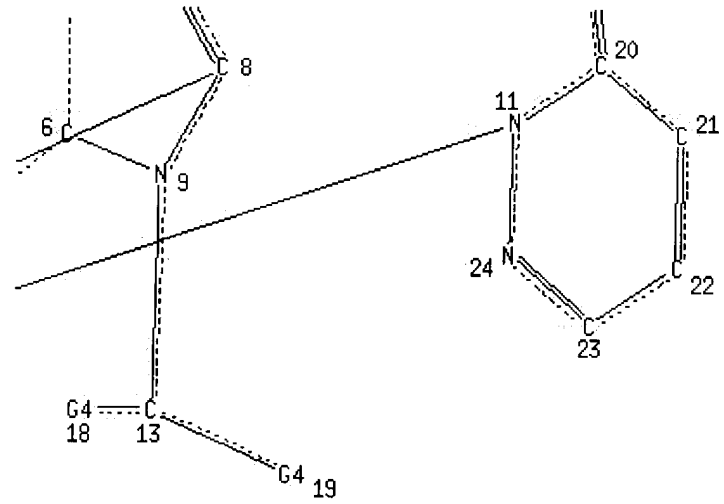
Page 1-A

10 C M2

Page 1-B



Page 2-A



Page 2-B

VAR G2=26/27/28
VAR G3=29/30
VAR G4=31/32
VAR G6=33/34
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:

HCOUNT	IS M2	AT	10
NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS C	AT	10
NSPEC	IS R	AT	11

```
NSPEC   IS C      AT  12
NSPEC   IS C      AT  13
NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
NSPEC   IS C      AT  16
NSPEC   IS C      AT  17
NSPEC   IS C      AT  18
NSPEC   IS C      AT  19
NSPEC   IS R      AT  20
NSPEC   IS R      AT  21
NSPEC   IS R      AT  22
NSPEC   IS R      AT  23
NSPEC   IS R      AT  24
NSPEC   IS C      AT  25
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  10 13 22 26 27 28 29 30 31 32 33 34
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   8
NUMBER OF NODES IS  34

STEREO ATTRIBUTES: NONE


=> s l32
SAMPLE SEARCH INITIATED 21:03:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      0 TO ITERATE

100.0% PROCESSED       0 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            0 TO        0
PROJECTED ANSWERS:               0 TO        0

L33           0 SEA SSS SAM L32

=> s l32 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 21:03:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      7 TO ITERATE

100.0% PROCESSED       7 ITERATIONS                                7 ANSWERS
SEARCH TIME: 00.00.01

L34           7 SEA SSS FUL L32

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             157.94    1282.38

FILE 'HCAPLUS' ENTERED AT 21:03:33 ON 14 MAR 2004
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FILE COVERS 1907 - 14 Mar 2004 VOL 140 ISS 12
FILE LAST UPDATED: 12 Mar 2004 (20040312/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l34
L35 4 L34

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.36	1284.74

FILE 'REGISTRY' ENTERED AT 21:03:40 ON 14 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES: 12 MAR 2004 HIGHEST RN 662722-88-5
DICTIONARY FILE UPDATES: 12 MAR 2004 HIGHEST RN 662722-88-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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L36 STRUCTURE UPLOADED

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L36 HAS NO ANSWERS
L36 STR

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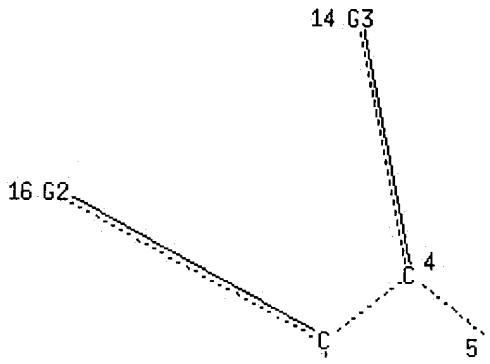
H 36 Ak 37

X 34 H 35

H 31 X 32 Ak 33



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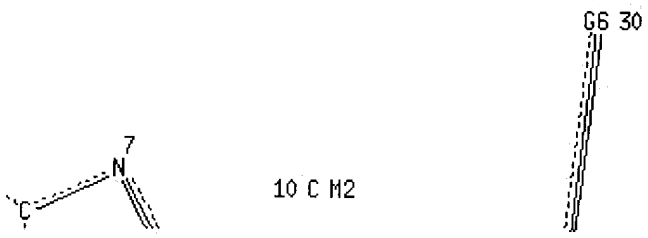

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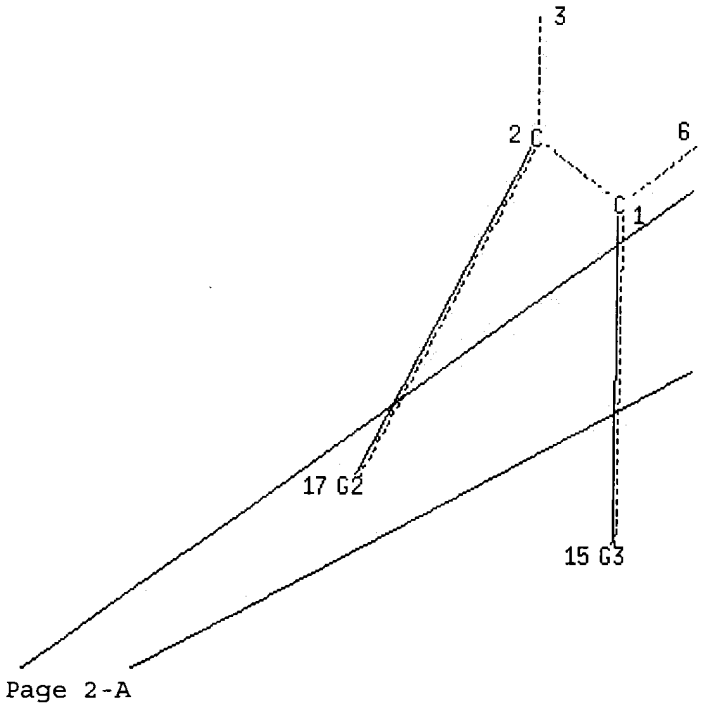

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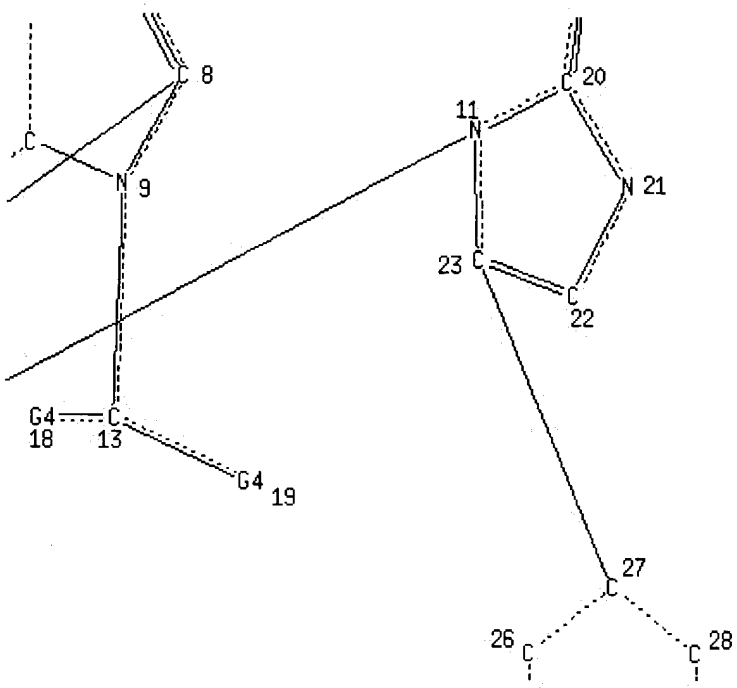

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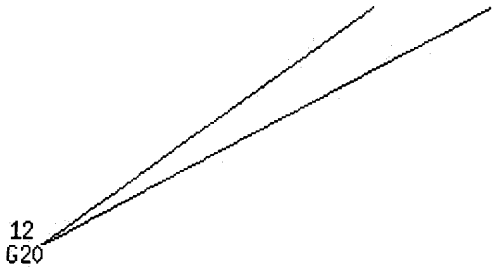

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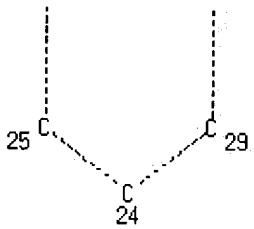

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VAR G4=36/37
VAR G6=38/39
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NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8

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MLEVEL  IS CLASS  AT  10 13 24 31 32 33 34 35 36 37 38 39
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  39

STEREO ATTRIBUTES: NONE


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SAMPLE SEARCH INITIATED 21:06:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      0 TO ITERATE

100.0% PROCESSED       0 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:             0 TO        0
PROJECTED ANSWERS:                0 TO        0

L37           0 SEA SSS SAM L36

=> s l36 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 21:06:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      3 TO ITERATE

100.0% PROCESSED       3 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

L38           3 SEA SSS FUL L36

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
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	ENTRY	SESSION
FULL ESTIMATED COST	157.10	1441.84

FILE 'HCAPLUS' ENTERED AT 21:06:22 ON 14 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 14 Mar 2004 VOL 140 ISS 12
FILE LAST UPDATED: 12 Mar 2004 (20040312/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L39             1 L38

=> d his

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L3              0 S L1 FULL
L4                STRUCTURE UPLOADED
L5              0 S L4
L6              0 S L4 FULL
L7                STRUCTURE UPLOADED
L8              0 S L7
L9              0 S L7 FULL
L10               STRUCTURE UPLOADED
L11            50 S L10
L12               STRUCTURE UPLOADED
L13            50 S L12
L14          2143 S L12 FULL

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L15           259 S L14

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L22           4 S L21

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L23           3 S L22

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L27          13 S L26

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L28             STRUCTURE UPLOADED
L29           4 S L28
L30          98 S L29 FULL

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L31          13 S L30

     FILE 'REGISTRY' ENTERED AT 20:59:25 ON 14 MAR 2004
L32             STRUCTURE UPLOADED
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L34           7 S L32 FULL

     FILE 'HCAPLUS' ENTERED AT 21:03:33 ON 14 MAR 2004
L35           4 S L34

     FILE 'REGISTRY' ENTERED AT 21:03:40 ON 14 MAR 2004
L36             STRUCTURE UPLOADED
L37           0 S L36
L38           3 S L36 FULL

     FILE 'HCAPLUS' ENTERED AT 21:06:22 ON 14 MAR 2004
L39           1 S L38

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          2553 YU, K?/AU
L40          4 L31 AND YU, K?/AU

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L40  ANSWER 1 OF 4  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

ACCESSION NUMBER: 2003:511082 HCAPLUS
DOCUMENT NUMBER: 139:85343
TITLE: Preparation of 2-(heterocyclylmethyl)benzimidazoles as respiratory syncytial virus antiviral agents
INVENTOR(S): **Yu, Kuo-long**; Wang, Xiangdong; Sun, Yaxiong; Cianci, Christopher; Thuring, Jan Willem; Combrink, Keith; Meanwell, Nicholas; Zhang, Yi; Civiello, Rita L.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 149 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053344	A2	20030703	WO 2002-US39220	20021206
WO 2003053344	A3	20031113		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003207868	A1	20031106	US 2002-309505	20021204

PRIORITY APPLN. INFO.: US 2001-339025P P 20011210
OTHER SOURCE(S): MARPAT 139:85343
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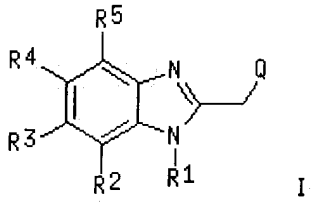

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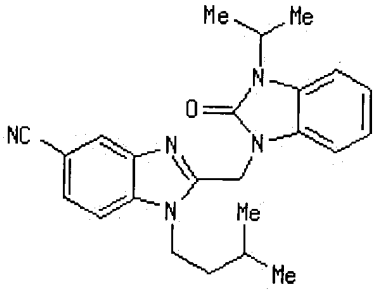


II

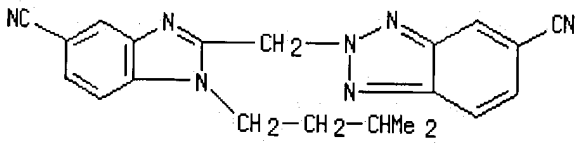
AB Title compds. I [wherein R1 = (CRaRb)nX; R2 = H; R3 = CONRhRi, CO2Rd, or (un)substituted alkyl; R4 = NH2, CONRhRi, heteroaryl, alkenyl, CO2Rd, N=CPh2, C(NOH)NH2, C(NH)NH2, or (un)substituted alkyl; R5 = CO2Rj or (un)substituted alkyl or alkenyl; Q = (un)substituted benzimidazolyl, benzotriazolyl, imidazopyridinyl, quinolinyl, quinazolinyl, benzyloxy, etc.; X = H or (un)substituted alkyl; Ra and Rb = independently H or (halo)alkyl; Rd = alkyl; Rh and Ri = independently H or alkyl; Rj = H or alkyl; n = 1-6; and pharmaceutically acceptable salts thereof] were prepd. as antiviral compds. More particularly, the invention provides 2-(heterocyclylmethyl)benzimidazole derivs. for the treatment of respiratory syncytial virus (RSV) infection. For example, 1-isopropyl-1,3-dihydrobenzimidazol-2-one was coupled with 2-chloromethyl-1-(3-methylbutyl)-1H-benzimidazole-5-carbonitrile in the presence of Cs2CO3 in DMF to give II (95%). Disclosed compds. protected HEp-2 cells from RSV-induced cytopathic effects with EC50 values between 50 μM and 0.001 μM, compared to an EC50 of 3 μM for ribavirin. I also displayed antiviral activity by reducing viral protein expression in HEp-2 cells with EC50 values between 50 μM and 0.001 μM, compared to an EC50 value of 3 μM for ribavirin. Thus, I and compns. comprising I are useful for the treatment of RSV infections.

IT **554457-35-1P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(antiviral agent; prepn. of (heterocyclylmethyl)benzimidazoles as RSV antiviral agents)

RN 554457-35-1 HCAPLUS

CN 2H-Benzotriazole-5-carbonitrile, 2-[[5-cyano-1-(3-methylbutyl)-1H-benzimidazol-2-yl]methyl]- (9CI) (CA INDEX NAME)



L40 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:442751 HCAPLUS

DOCUMENT NUMBER: 139:159456

TITLE: Fundamental structure-activity relationships associated with a new structural class of respiratory syncytial virus inhibitor

AUTHOR(S): **Yu, Kuo-Long**; Zhang, Yi; Civiello, Rita L.; Kadow, Kathleen F.; Cianci, Christopher; Krystal, Mark; Meanwell, Nicholas A.

CORPORATE SOURCE: Department of Chemistry, The Bristol-Myers Squibb Pharmaceutical Research Institute, Wallingford, CT, 06492, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(13), 2141-2144
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

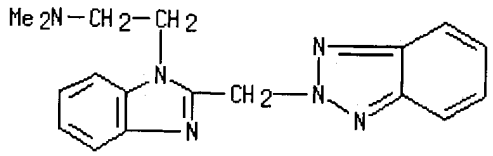
OTHER SOURCE(S): CASREACT 139:159456

AB Structure-activity relationships surrounding the dialkylamino side chain of a series of benzotriazole-derived inhibitors of respiratory syncytial virus fusion were examd. The results indicate that the topol. of the side chain is important but the terminus element offers considerable latitude to modulate phys. properties.

IT **5823-63-2**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fundamental structure-activity relationships assocd. with a new structural class of respiratory syncytial virus inhibitor)

RN 5823-63-2 HCAPLUS

CN 1H-Benzimidazole-1-ethanamine, 2-(2H-benzotriazol-2-ylmethyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L40 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:556140 HCAPLUS
DOCUMENT NUMBER: 137:125159
TITLE: Preparation and antiviral activity of heterocyclic substituted 2-methylbenzimidazole antiviral agents
INVENTOR(S): **Yu, Kuo-Long**; Civiello, Rita L.; Combrink, Keith D.; Gulgeze, Hatice Belgin; Sin, Ny; Wang, Xiangdong; Meanwell, Nicholas; Venables, Brian Lee; Zhang, Yi; Pearce, Bradley C.; Yin, Zhiwei; Thuring, Jan Willem
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 89 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002099208	A1	20020725	US 2001-994012	20011116
WO 2002062290	A2	20020815	WO 2001-US45149	20011120
WO 2002062290	A3	20021121		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1343499	A2	20030917	EP 2001-270116	20011120

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRIORITY APPLN. INFO.:
US 2000-257139P P 20001220
WO 2001-US45149 W 20011120

OTHER SOURCE(S): MARPAT 137:125159
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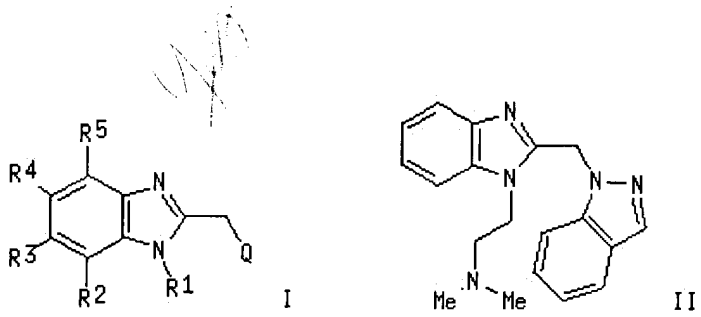


I II

AB The title compds. [I; R1 = (CRaRb)nX; Ra, Rb = independently H, C1-6 (un)substituted alkyl; X = H, C1-6 (un)substituted alkyl; n = 1-6; R2, R5 = independently H or halogen; R3, R4 = independently H, halogen, C1-6 (un)substituted alkyl; Q = heterocyclic group], useful in the treatment of viral infections, more particularly, for the treatment of respiratory syncytial virus infection, were prepd. E.g., a four-step synthesis of II, starting with 2-(chloromethyl)benzimidazole, was given. The antiviral

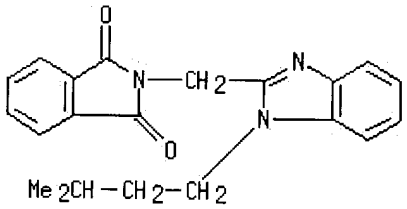
activity of these compds. against respiratory syncytial virus (RSV) was detd. in HEp-2 (ATCC CCL 23) cells. The title compds. I, disclosed herein, show antiviral activity with EC50s between 50 μM and 0.001 μM.

IT **443985-58-8P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. and use of heterocyclic substituted 2-methyl-benzimidazole antiviral agents)

RN 443985-58-8 HCAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[[1-(3-methylbutyl)-1H-benzimidazol-2-yl]methyl]- (9CI) (CA INDEX NAME)



L40 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:84617 HCAPLUS
DOCUMENT NUMBER: 132:122625
TITLE: Preparation of substituted benzimidazole antiviral agents
INVENTOR(S): **Yu, Kuo-long**; Civiello, Rita Lee; Krystal, Mark R.; Kadow, Kathleen F.; Meanwell, Nicholas A.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000004900	A1	20000203	WO 1999-US12398	19990720
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CA 2338147	AA	20000203	CA 1999-2338147	19990720
AU 9950809	A1	20000214	AU 1999-50809	19990720
AU 741946	B2	20011213		
EP 1098644	A1	20010516	EP 1999-935302	19990720
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002521334	T2	20020716	JP 2000-560893	19990720

US 2003139450 A1 20030724 US 2002-289829 20021107
PRIORITY APPLN. INFO.: US 1998-93387P P 19980720
US 1999-354958 B1 19990716
WO 1999-US12398 W 19990720
OTHER SOURCE(S): MARPAT 132:122625
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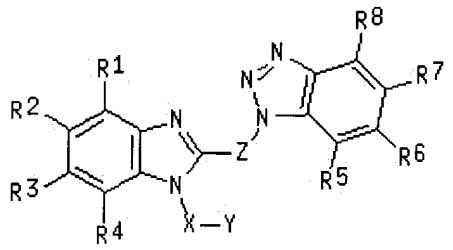

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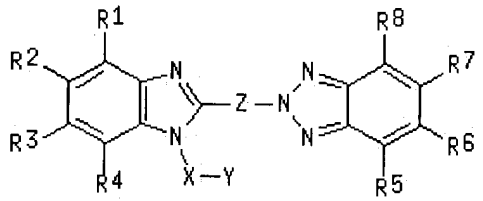

II

AB The title compds. [I and II; R1-R8 = H, alkyl, NO2, etc.; X = straight, branched or cyclic C2-12 alkyl, alkenyl, alkynyl; Y = (un)substituted Ph, dioxolane, pyridine, etc.; XY = CH2Ph, CH2COPh, CH2CHOHPh, etc.; Z = (CR12R13)n; n = 1-4; R12, R13 = H, straight, branched or cyclic alkyl], useful in the treatment of viral infections, particularly, for the treatment of respiratory syncytial virus infection, were prepd. Thus, coupling 1-(1H-benzimidazol-2-ylmethyl)-1H-benzotriazole with 2-dimethylaminoethyl chloride hydrochloride in the presence of NaH in THF afforded 23% I [Z = CH2: XY = (CH2)2NMe2; R1-R8 = H] which showed 100% HEp-2 cell protection against RSV at 4 μg/mL.

IT **5823-63-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of substituted benzimidazole antiviral agents)

RN 5823-63-2 HCAPLUS
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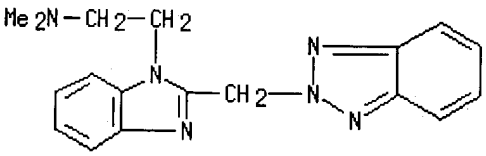

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

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     (FILE 'HOME' ENTERED AT 20:35:55 ON 14 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 20:36:00 ON 14 MAR 2004
L1                STRUCTURE UPLOADED
L2              0 S L1
L3              0 S L1 FULL
L4                STRUCTURE UPLOADED
L5              0 S L4
L6              0 S L4 FULL
L7                STRUCTURE UPLOADED
L8              0 S L7
L9              0 S L7 FULL
L10               STRUCTURE UPLOADED
L11            50 S L10
L12               STRUCTURE UPLOADED
L13            50 S L12
L14          2143 S L12 FULL

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L15           259 S L14

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L16               STRUCTURE UPLOADED
L17            50 S L16
L18          1605 S L16 FULL

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L19           210 S L18
L20           183 S L19 AND PD < JANUARY 2001
L21               STRUCTURE UPLOADED
                  S L21

     FILE 'REGISTRY' ENTERED AT 20:56:20 ON 14 MAR 2004
L22             4 S L21

     FILE 'HCAPLUS' ENTERED AT 20:56:21 ON 14 MAR 2004
L23             3 S L22

     FILE 'REGISTRY' ENTERED AT 20:56:27 ON 14 MAR 2004
L24               STRUCTURE UPLOADED
L25             4 S L24
L26            98 S L24 FULL

     FILE 'HCAPLUS' ENTERED AT 20:56:54 ON 14 MAR 2004
L27            13 S L26

     FILE 'REGISTRY' ENTERED AT 20:57:08 ON 14 MAR 2004
L28               STRUCTURE UPLOADED
L29             4 S L28
L30            98 S L29 FULL

     FILE 'HCAPLUS' ENTERED AT 20:59:15 ON 14 MAR 2004
L31            13 S L30

     FILE 'REGISTRY' ENTERED AT 20:59:25 ON 14 MAR 2004
L32               STRUCTURE UPLOADED
L33             0 S L32
L34             7 S L32 FULL
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L35            4 S L34

     FILE 'REGISTRY' ENTERED AT 21:03:40 ON 14 MAR 2004
L36              STRUCTURE UPLOADED
L37            0 S L36
L38            3 S L36 FULL

     FILE 'HCAPLUS' ENTERED AT 21:06:22 ON 14 MAR 2004
L39            1 S L38
L40            4 S L31 AND YU, K?/AU

=> s l31 not l40
L41            9 L31 NOT L40

=> d l41, ibib abs fhitstr, 1-9

L41  ANSWER 1 OF 9  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

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ACCESSION NUMBER:          2002:888718  HCAPLUS
DOCUMENT NUMBER:           137:384842
TITLE:                     Benzimidazole compounds and antiviral uses thereof
INVENTOR(S):               Lackey, John William; Kinder, Daniel S.; Tvermoes,
                           Nicolai A.
PATENT ASSIGNEE(S):        Trimeris, Inc., USA
SOURCE:                    PCT Int. Appl., 143 pp.
                           CODEN: PIXXD2
DOCUMENT TYPE:             Patent
LANGUAGE:                  English
FAMILY ACC. NUM. COUNT:    1
PATENT INFORMATION:

     PATENT NO.         KIND  DATE          APPLICATION NO.  DATE
     ---------------    ----  --------      ---------------  --------
     WO 2002092575       A1   20021121      WO 2002-US14598  20020510
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
            CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2003119754       A1   20030626      US 2002-141839   20020509
PRIORITY APPLN. INFO.:                     US 2001-290038P  P  20010511
OTHER SOURCE(S):           MARPAT 137:384842
GI
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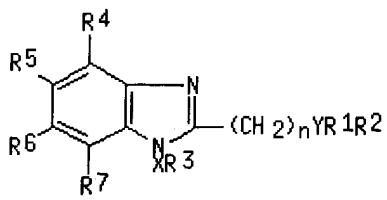

I

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AB   Title compds. I [R1, R2 = H, (un)substituted alkyl, cycloalkyl,
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heterocyclic, aryl, heteroaryl; R3 = H, halo, (un)substituted alkyl, Oh, alkoxy, aryl, heterocyclic, heteroaryl; R4-R7 = H, halo, (un)substituted alkyl, OH, alkoxy, aryl, heterocyclic, heteroaryl; X = bond, (un)substituted alkylene, C:N, CO, P, S; Y = N, P, O, S; when Y = O, S, R2 is absent; n = 0-4] were prepd. for use as virucides that inhibit membrane fusion assocd. events such as viral transmission, reduce viral load or otherwise treat viral infections, particularly that caused by Respiratory Syncytial Virus. Thus, I [R1 = cyclohexyl, R2 = CHMe2, Y = N, X = CH2, R3 = 2-quinolinyl, R4-R7 = H] had IC50 of 5.16 μg/mL.

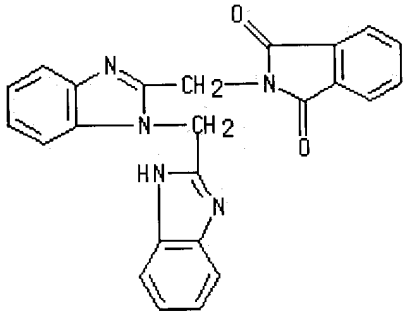
IT **475648-38-5P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazole derivs. as virucides for treating Respiratory Syncytial Virus infections)

RN 475648-38-5 HCAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[[1-(1H-benzimidazol-2-ylmethyl)-1H-benzimidazol-2-yl]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:841902 HCAPLUS
DOCUMENT NUMBER: 133:362969
TITLE: Synthesis of heterocyclic derivs. of N-(phenylcyclohexylcarbonyl)phenylglycine amide for treatment of cardiovascular ischemia
INVENTOR(S): Bischoff, Erwin; Lensky, Stephan; Muller, Stephan Nicholas; Paulsen, Holger; Keldenich, Jorg; Krahn, Thomas; Schuhmacher, Joachim
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 30 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19924819	A1	20001130	DE 1999-19924819	19990529
WO 2000073274	A2	20001207	WO 2000-EP4431	20000516
WO 2000073274	A3	20010419		

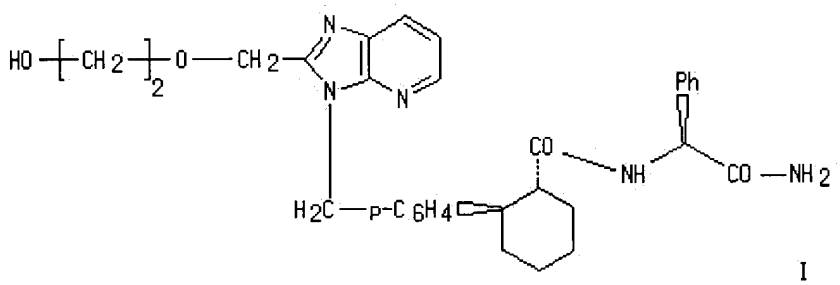
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,

ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA,
ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

BR 2000011049	A	20020319	BR 2000-11049	20000516
EP 1187812	A2	20020320	EP 2000-925290	20000516
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003500474	T2	20030107	JP 2000-621340	20000516
AU 766140	B2	20031009	AU 2000-44057	20000516
ZA 2001008894	A	20021029	ZA 2001-8894	20011029

PRIORITY APPLN. INFO.: DE 1999-19924819 A 19990529
WO 2000-EP4431 W 20000516

OTHER SOURCE(S): MARPAT 133:362969
GI



I

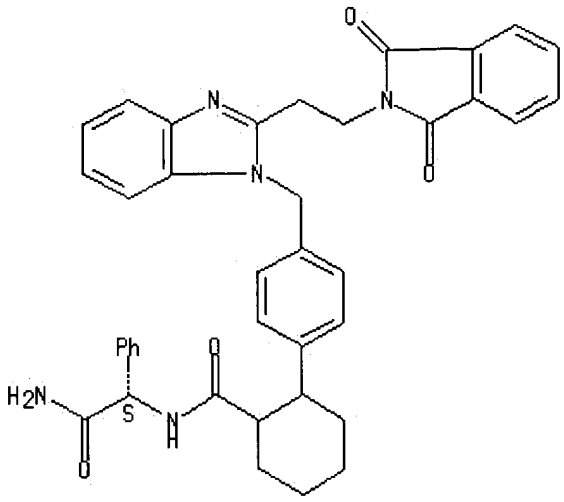
AB Title compds., e.g. (I), were prepd. for use in treating cardiovascular ischemic disorders in humans or animals. Thus, 2-(2-hydroxyethoxymethyl)pyrido[2,3-d]imidazole (prepn. given) was reacted with (1R,2R)-2-(4-methylphenyl)cyclohexanecarboxylic acid (resoln. from racemate given) to yield the intermediate material which was reacted with (S)-phenylglycinamide hydrochloride to give I. In in vitro tests of rabbit erythrocyte adenosine uptake, the 2-(morpholin-4-yl)methyl [in place of the 2-(2-hydroxyethoxymethyl) sidechain] compd. had IC50 of 15 nM; the 2-(piperazinyl)benzimidazolyl variant had IC50 of 25 nM.

IT **307931-40-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of heterocyclic derivs. of N-(phenylcyclohexylcarbonyl)phenylglycine amide for treatment of cardiovascular ischemia)

RN 307931-40-4 HCAPLUS

CN Benzeneacetamide, α-[[[2-[4-[[2-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]-1H-benzimidazol-1-yl]methyl]phenyl]cyclohexyl]carbonyl]amino]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L41 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:841901 HCAPLUS
DOCUMENT NUMBER: 133:362968
TITLE: Synthesis of heterocyclic derivs. of N-(phenylcyclohexylcarbonyl)phenylglycine amide for treatment of cerebral ischemia or injury
INVENTOR(S): Freund, Wolf-Dietrich; Lensky, Stephan; Muller, Stephan Nicholas; Paulsen, Holger; Keldenich, Jorg; Horvath, Ervin; Schuhmacher, Joachim
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 30 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19924818	A1	20001130	DE 1999-19924818	19990529
WO 2000073275	A1	20001207	WO 2000-EP4417	20000516
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 2000011061	A	20020305	BR 2000-11061	20000516
EP 1185516	A1	20020313	EP 2000-925288	20000516
EP 1185516	B1	20030502		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003500475	T2	20030107	JP 2000-621341	20000516
EE 200100634	A	20030217	EE 2001-634	20000516
AT 238997	E	20030515	AT 2000-925288	20000516
AU 765752	B2	20030925	AU 2000-44055	20000516
PT 1185516	T	20030930	PT 2000-925288	20000516

ES 2197870	T3	20040116	ES 2000-925288	20000516
ZA 2001009263	A	20021111	ZA 2001-9263	20011109
BG 106107	A	20020531	BG 2001-106107	20011113
NO 2001005810	A	20020125	NO 2001-5810	20011128
HR 2001000955	A1	20030831	HR 2001-955	20011224

PRIORITY APPLN. INFO.: DE 1999-19924818 A 19990529
WO 2000-EP4417 W 20000516

OTHER SOURCE(S): MARPAT 133:362968
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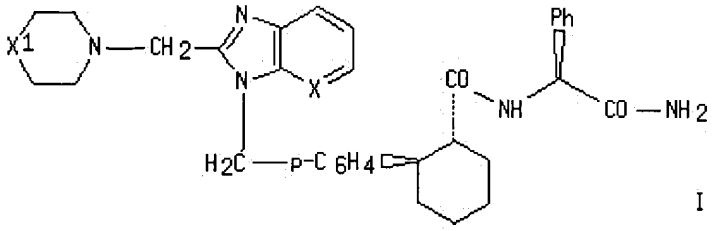


I

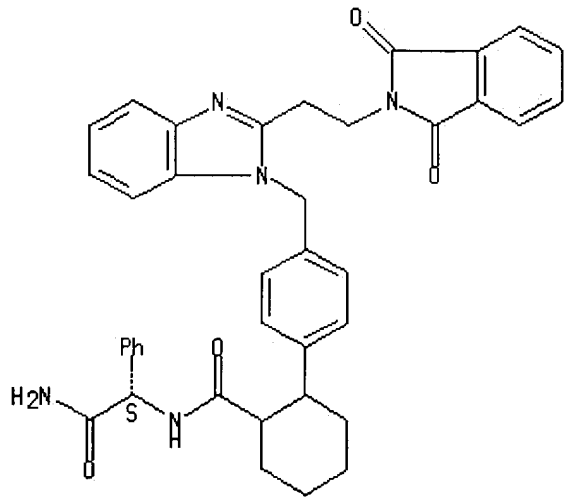
AB Title compds., e.g. I, were prepd. for use in treating ischemic brain diseases in humans or animals. Thus I [X = N, X1 = O (II)] was prepd. in six steps, starting from 2,3-diaminopyridine, glycolic acid, (1R,2R)-2-(4-bromomethylphenyl)cyclohexane-1-carboxylic acid tert-Bu ester (prepn. given), and (S)-phenylglycinamide hydrochloride. Similarly prepd. was I [X = C, X1 = N(Me) (III)]. In in vivo (binding of calf cortex adenosine transport protein) compds. II and III had Ki = 2 nM. In in vitro tests of rat brain reperfusion injury, II and III were effective at 0.001 mg/kg, reducing infarct vol. 81-91% of control.

IT **307931-40-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of heterocyclic derivs. of N-(phenylcyclohexylcarbonyl)phenylglycine amide for treatment of cerebral ischemia or injury)

RN 307931-40-4 HCAPLUS

CN Benzeneacetamide, α-[[[2-[4-[[2-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]-1H-benzimidazol-1-yl]methyl]phenyl]cyclohexyl]carbonyl]amino]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L41 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

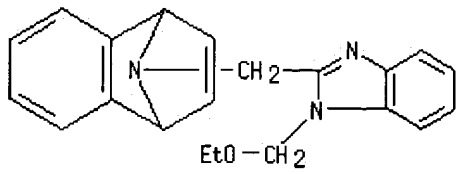
ACCESSION NUMBER: 1995:842837 HCAPLUS
DOCUMENT NUMBER: 123:274303
TITLE: Synthesis of New Types of Dithiolene Ligands
AUTHOR(S): Tian, Zong-Qiang; Donahue, James P.; Holm, R. H.
CORPORATE SOURCE: Department of Chemistry, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Inorganic Chemistry (1995), 34(22), 5567-72
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Three new types of dithiolene ligands were prepd. from Diels-Alder reactions of the diene 2,3-bis(benzylthio)-1,4-dichloro-5,5-dimethoxy-1,3-cyclopentadiene (4), whose structure was established by an x-ray detn. Reaction of 4 with excess norbornadiene as the dienophile affords I, S-deprotection and dechlorination of which with Na in liq. NH3 lead to the ligand salt Na2(L-S2) (6). Treatment of 2 equiv of 4 with 1 equiv of norbornadiene gives the tetraprotected bis(dithiolene) II, which is converted to the ligand salt Na4(L-S4) (8) by Na in liq. NH3. Reaction of 2-(chloromethyl)-1-(ethoxymethyl)benzimidazole with 1,4-dihydronaphthalen-1,4-imine gives the N-substituted imine dienophile III. Reaction of the latter with 4 produces the adduct IV, which after deprotection affords the ligand salt Na2(L-NS2) (12). The endo,exo ligand stereochem. outcome of the Diels-Alder reaction was proven by detn. of the structure of [Ni(L-S2)2] (13). 13 Crystallizes in monoclinic space group P21/n with a 7.636(2), b 8.64(4), c 20.962(4) Å, β 96.57(2)°, and Z = 2. The complex is planar and centrosym. The related complex [Ni(L-S2)(dppe)]·Et2O was isolated in triclinic point group P.hivin.1 with a 11.087(5), b 13.173(7), c 15.663(6) Å, α 90.82(5), β 97.49(3), γ 114.60(3)°, and Z = 2. Also prepd. were [Pd(L-S2)(bpy)] and [Mo(L-S2)3]. The ligand L-S2 is the 1st dithiolene with structure above and below the chelate ring. This feature does not hinder the formation of bis and tris complexes; the collective properties of the four complexes indicate that L-S2 is a generic dithiolene with electron-releasing substituents. The endo,exo stereochem. of L-S4 was proven by a crystal structure detn. of II. This ligand is a bis(dithiolene) capable of forming binuclear complexes with multielectron redox capacity. The endo,exo stereochem. of L-NS2 was demonstrated by the x-ray structure of IV. This species is designed as a facial tridentate ligand; the method of synthesis is such that the benzimidazole ligand should be replaceable by other binding groups.

IT **168915-36-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and Diels-Alder reaction of)

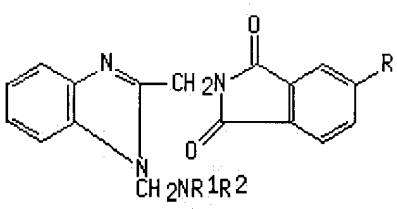
RN 168915-36-4 HCAPLUS
CN Naphthalen-1,4-imine, 9-[[1-(ethoxymethyl)-1H-benzimidazol-2-yl]methyl]-1,4-dihydro- (9CI) (CA INDEX NAME)



L41 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

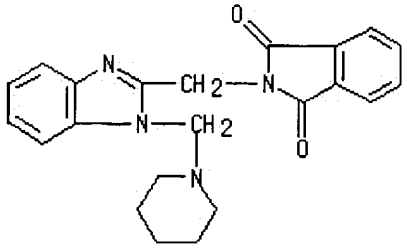
ACCESSION NUMBER: 1988:447836 HCAPLUS
DOCUMENT NUMBER: 109:47836
TITLE: Synthesis and pharmacological screening of 1-(substituted aminomethyl)2-(5-substituted phthalimidomethyl)benzimidazoles
AUTHOR(S): Agarwal, Sunita; Pande, Alka; Swarup, Sanjay; Saxena, V. K.; Chowdhury, S. R.
CORPORATE SOURCE: Dep. Chem., Lucknow Univ., Lucknow, 226 007, India
SOURCE: Indian Drugs (1988), 25(6), 229-35
CODEN: INDRBA; ISSN: 0019-462X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A series of 20 title compds. (I, R = H, NO2; R1 and R2 = alkyl, aryl; NR1R2 = heterocyclic) was prepd. by reactions of aminomethylbenzimidazole with phthalic anhydrides followed by Mannich reactions. I were tested for toxicity, cardiovascular, anti-inflammatory, and central nervous activity in cats and other models. All I had low toxicity with LD50 >1 g/kg. I (R = H) had mild cardiovascular effects. Max. anti-inflammatory effect was obsd. with I (R = NO2; R1 = R2 = Me). Several I (R = H) had depressant or stimulatory effects, while all I (R = NO2) had some stimulant activity.

IT **115398-74-8P**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(prepn. and pharmacol. of, structure in relation to)
RN 115398-74-8 HCAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[[1-(1-piperidinylmethyl)-1H-benzimidazol-2-yl]methyl]- (9CI) (CA INDEX NAME)



L41 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1983:107243 HCAPLUS
DOCUMENT NUMBER: 98:107243
TITLE: Synthesis of some new benzimidazoles as antiamebic agents
AUTHOR(S): Misra, Vinay S.; Shah, Pramilla; Saxena, V. K.
CORPORATE SOURCE: Dep. Chem., Univ. Lucknow, Lucknow, 226 007, India
SOURCE: Journal of the Indian Chemical Society (1982), 59(9), 1074-6
CODEN: JICSAH; ISSN: 0019-4522
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 98:107243
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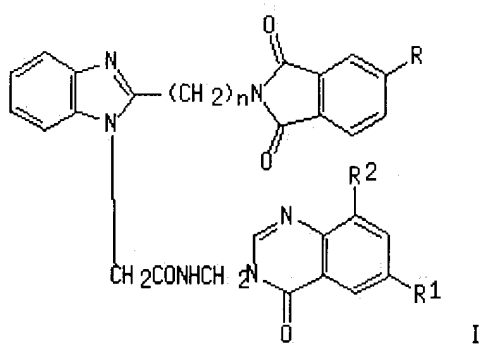
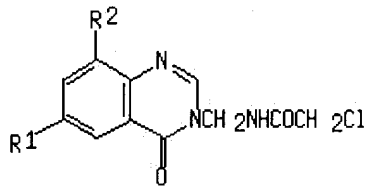


I



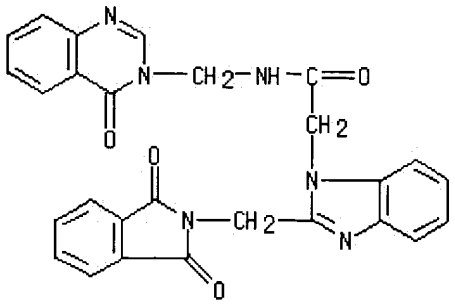
II

AB Fourteen benzimidazole derivs. I (R = H, NO2; R1 = H, Br, NO2; R2 = H, Br, n = 1, 2) were prepd. by treating 2-(aminoalkyl)benzimidazoles with phthalic anhydride followed by reaction with the quinazoline derivs. II. Some I show significant antiamebic activity in vitro against Entamoeba histolytica at 125 μg/mL.

IT **84900-10-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and amebicidal activity of)

RN 84900-10-7 HCAPLUS

CN 1H-Benzimidazole-1-acetamide, 2-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]-N-[(4-oxo-3(4H)-quinazolinyl)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)

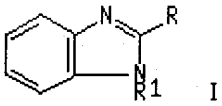


2 HCl

L41 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

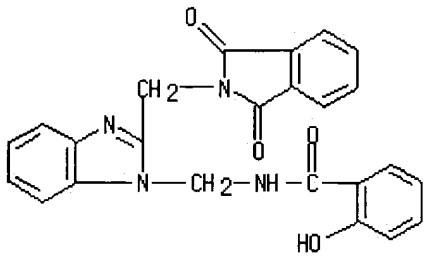
ACCESSION NUMBER: 1979:6303 HCAPLUS
DOCUMENT NUMBER: 90:6303
TITLE: Possible antifertility compounds. Part II: Synthesis of 1, 2-disubstituted benzimidazoles
AUTHOR(S): Tiwari, S. S.; Upreti, Amrapali
CORPORATE SOURCE: Dep. Chem., Univ. Lucknow, Lucknow, India
SOURCE: Journal of the Indian Chemical Society (1978), 55(3), 272-4
CODEN: JICSAH; ISSN: 0019-4522
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Ten new benzimidazole derivs., I (R = 2-methylphthalimido, 3,5-(O2N)2C6H4CONHCH2, α-phthalimidoethyl, etc.; R1 = H) were prepd. by condensation of o-(H2N)2C6H4 with N-substituted amino acids. Some I (R = H) were subjected to Mannich-type condensation to yield I (R1 = o-HOC6H4CONHCH2). Two compds. were tested for antiestrogenic activity and one was evaluated as a male antifertility agent but they was found to be ineffective.

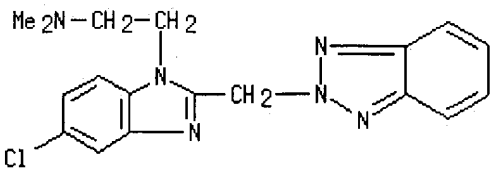
IT **68501-77-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 68501-77-9 HCAPLUS
CN Benzamide, N-[[2-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl]-1H-benzimidazol-1-yl]methyl]-2-hydroxy- (9CI) (CA INDEX NAME)



L41 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1975:514300 HCAPLUS
DOCUMENT NUMBER: 83:114300
TITLE: Dialkylaminoalkylbenzimidazoles of pharmacological interest. IV
AUTHOR(S): Paglietti, G.; Boido, V.; Sparatore, F.
CORPORATE SOURCE: Ist. Chim. Farm. Tossicol., Univ. Napoli, Naples, Italy
SOURCE: Farmaco, Edizione Scientifica (1975), 30(6), 505-11
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Italian
OTHER SOURCE(S): CASREACT 83:114300
GI For diagram(s), see printed CA Issue.
AB Analgesic benzimidazolylmethylbenzotriazoles I and II (R = Cl, CF3, Ac, NO2; R1 = (CH2)nNMe2, (CH2)nNEt2, lupinyl; n = 2, 3) were prepd. by treating 4,2-R(H2N)C6H3NHR1 with benzotriazolylacetic acids.
IT **56756-43-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 56756-43-5 HCAPLUS
CN 1H-Benzimidazole-1-ethanamine, 2-(2H-benzotriazol-2-ylmethyl)-5-chloro-N,N-dimethyl- (9CI) (CA INDEX NAME)



L41 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1966:35864 HCAPLUS
DOCUMENT NUMBER: 64:35864
ORIGINAL REFERENCE NO.: 64:6645g-h,6646a-c
TITLE: Benzotriazolylalkyl benzimidazoles and their dialkylaminoalkyl derivatives
AUTHOR(S): Pagani, F.; Sparatore, F.
CORPORATE SOURCE: Univ. Genoa, Italy
SOURCE: Bollettino Chimico Farmaceutico (1965), 104(7), 427-31
CODEN: BCFAAI; ISSN: 0006-6648
DOCUMENT TYPE: Journal
LANGUAGE: Italian
GI For diagram(s), see printed CA Issue.
AB The prepn. of benzimidazole derivs. of the general formulas I or II was

described. A mixt. of 0.022 mole o-phenylenediamine and 0.02 mole of the corresponding benzotriazolylacetic, propionic, or butyric acid was heated in an oil bath at 180-5° during 1 hr.; the cooled mass was powd., stirred 1 hr. with 100 ml. 2N Na2CO3, the ppt. filtered off, washed with H2O, crystd. with C from boiling EtOH, to give 50-87% I or II (R = H) (type, n, and m.p. given): I, 1,209-10°; I, 2, 209-10°; I, 3, 104-5°; II, 1,200-1°; II, 2, 194-5°; II, 3, 144-5°. The alkylation of I or II (n = 1) was made according to one of the following methods. (a) To a cooled and stirred soln. of 5 g. I or II in 20 ml. HCONMe2, 1 g. powd. NaNH2 was added under N; the mixt. was heated 1 hr. at 40-5°, 0.024 mole of the corresponding dialkylaminoalkyl chloride in 5 ml. HCONMe2 was added, the mixt. kept, with stirring under N, at 40-5° during 24 hrs., filtered, the solvent and excess dialkylaminoalkyl chloride evapd. in vacuo, the residue washed with Et2O-petr. ether (1:1), extd. several times with boiling anhyd. Et2O, the ethereal soln. concd., cooled, and filtered, the filtrate evapd. to dryness, the residue taken up in 75 ml. 0.2N HCl, the soln. filtered, the filtrate alkalinized with 2N Na2CO3, extd. with Et2O, and the ethereal soln. worked up to give 40-70% of the corresponding alkyl deriv., which was crystd. in Et2O-petr. ether. (b) To the reaction mixt. of 2.5 g. I or II (n = 1)(dissolved in 15 ml. HCONMe2) and 0.47 g. NaNH2, prepd. as above, 2.1 g. chlorolupinane was added, the mixt. heated in an oil bath at 140-5° for 3 hrs., filtered hot, evapd. to dryness, and the residue crystd. in C6H6 (Ia) or anhyd. Et2O (IIa), with 68% and 62% yield, resp. The following alkyl derivs. were prepd. (n = 1) (type, R, and m.p. given): I, (CH2)2NMe2, 124-5°; I, (CH2)2NEt2, 95-7°; I, (CH2)3NMe2, 103-4°; I, (CH2)3NEt2, 79-81°; I, α-lupinanyl (Ia), 198-9°; II, (CH2)2NMe2, 37-40°; II, (CH2)2NEt2, -- (picrate m. 205-6°); II, (CH2)3NMe2, --(picrate m. 213-14°); II, (CH2)3NEt2, -- (picrate m. 178-81°); II, α-lupinanyl (IIa), 157-8°. These compds. were considered as potential analgesics.

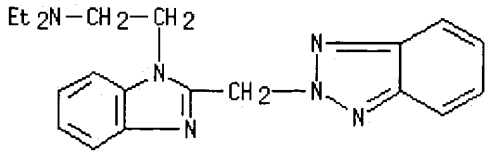
IT **5823-64-3**, 2H-Benzotriazole, 2-[[1-[2-(diethylamino)ethyl]-2-benzimidazolyl]methyl], picrate
(prepn. of)

RN 5823-64-3 HCAPLUS

CN 2H-Benzotriazole, 2-[[1-[2-(diethylamino)-ethyl]-2-benzimidazolyl]methyl]-, picrate (7CI, 8CI) (CA INDEX NAME)

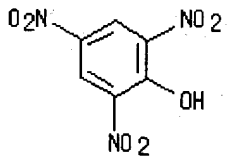
CM 1

CRN 5914-83-0
CMF C20 H24 N6



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7

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=> d his

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     FILE 'REGISTRY' ENTERED AT 20:36:00 ON 14 MAR 2004
L1                STRUCTURE UPLOADED
L2              0 S L1
L3              0 S L1 FULL
L4                STRUCTURE UPLOADED
L5              0 S L4
L6              0 S L4 FULL
L7                STRUCTURE UPLOADED
L8              0 S L7
L9              0 S L7 FULL
L10               STRUCTURE UPLOADED
L11            50 S L10
L12               STRUCTURE UPLOADED
L13            50 S L12
L14          2143 S L12 FULL

     FILE 'HCAPLUS' ENTERED AT 20:48:14 ON 14 MAR 2004
L15           259 S L14

     FILE 'REGISTRY' ENTERED AT 20:48:25 ON 14 MAR 2004
L16               STRUCTURE UPLOADED
L17            50 S L16
L18          1605 S L16 FULL

     FILE 'HCAPLUS' ENTERED AT 20:52:42 ON 14 MAR 2004
L19           210 S L18
L20           183 S L19 AND PD < JANUARY 2001
L21               STRUCTURE UPLOADED
                  S L21

     FILE 'REGISTRY' ENTERED AT 20:56:20 ON 14 MAR 2004
L22             4 S L21

     FILE 'HCAPLUS' ENTERED AT 20:56:21 ON 14 MAR 2004
L23             3 S L22

     FILE 'REGISTRY' ENTERED AT 20:56:27 ON 14 MAR 2004
L24               STRUCTURE UPLOADED
L25             4 S L24
L26            98 S L24 FULL

     FILE 'HCAPLUS' ENTERED AT 20:56:54 ON 14 MAR 2004
L27            13 S L26

     FILE 'REGISTRY' ENTERED AT 20:57:08 ON 14 MAR 2004
L28               STRUCTURE UPLOADED
L29             4 S L28
L30            98 S L29 FULL
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     FILE 'HCAPLUS' ENTERED AT 20:59:15 ON 14 MAR 2004
L31            13 S L30

     FILE 'REGISTRY' ENTERED AT 20:59:25 ON 14 MAR 2004
L32               STRUCTURE UPLOADED
L33             0 S L32
L34             7 S L32 FULL

     FILE 'HCAPLUS' ENTERED AT 21:03:33 ON 14 MAR 2004
L35             4 S L34

     FILE 'REGISTRY' ENTERED AT 21:03:40 ON 14 MAR 2004
L36               STRUCTURE UPLOADED
L37             0 S L36
L38             3 S L36 FULL

     FILE 'HCAPLUS' ENTERED AT 21:06:22 ON 14 MAR 2004
L39             1 S L38
L40             4 S L31 AND YU, K?/AU
L41             9 S L31 NOT L40

=> d 135 and yu, k?/au
'K?' MUST END IN '/Q', '/A', '/L', '/S' OR '/B'
The saved name for a query (or structure or screen set) must end with
'/Q'.  The saved name for an answer set must end with '/A'.  The saved
name for an L# list must end with '/L'.  SDI request names must end
with '/S'.  To see a list of all saved query, answer set,, and L# list
names for this loginid, enter "DISPLAY SAVED" at an arrow
prompt (=>).  Enter "DISPLAY SAVED/S" to see a list of SDI request
names.  Enter "DISPLAY SAVED/B" to see a list of BATCH search
requests.

=> d his

     (FILE 'HOME' ENTERED AT 20:35:55 ON 14 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 20:36:00 ON 14 MAR 2004
L1                STRUCTURE UPLOADED
L2              0 S L1
L3              0 S L1 FULL
L4                STRUCTURE UPLOADED
L5              0 S L4
L6              0 S L4 FULL
L7                STRUCTURE UPLOADED
L8              0 S L7
L9              0 S L7 FULL
L10               STRUCTURE UPLOADED
L11            50 S L10
L12               STRUCTURE UPLOADED
L13            50 S L12
L14          2143 S L12 FULL

     FILE 'HCAPLUS' ENTERED AT 20:48:14 ON 14 MAR 2004
L15           259 S L14

     FILE 'REGISTRY' ENTERED AT 20:48:25 ON 14 MAR 2004
L16               STRUCTURE UPLOADED
L17            50 S L16
L18          1605 S L16 FULL
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     FILE 'HCAPLUS' ENTERED AT 20:52:42 ON 14 MAR 2004
L19          210 S L18
L20          183 S L19 AND PD < JANUARY 2001
L21              STRUCTURE UPLOADED
                 S L21

     FILE 'REGISTRY' ENTERED AT 20:56:20 ON 14 MAR 2004
L22            4 S L21

     FILE 'HCAPLUS' ENTERED AT 20:56:21 ON 14 MAR 2004
L23            3 S L22

     FILE 'REGISTRY' ENTERED AT 20:56:27 ON 14 MAR 2004
L24              STRUCTURE UPLOADED
L25            4 S L24
L26           98 S L24 FULL

     FILE 'HCAPLUS' ENTERED AT 20:56:54 ON 14 MAR 2004
L27           13 S L26

     FILE 'REGISTRY' ENTERED AT 20:57:08 ON 14 MAR 2004
L28              STRUCTURE UPLOADED
L29            4 S L28
L30           98 S L29 FULL

     FILE 'HCAPLUS' ENTERED AT 20:59:15 ON 14 MAR 2004
L31           13 S L30

     FILE 'REGISTRY' ENTERED AT 20:59:25 ON 14 MAR 2004
L32              STRUCTURE UPLOADED
L33            0 S L32
L34            7 S L32 FULL

     FILE 'HCAPLUS' ENTERED AT 21:03:33 ON 14 MAR 2004
L35            4 S L34

     FILE 'REGISTRY' ENTERED AT 21:03:40 ON 14 MAR 2004
L36              STRUCTURE UPLOADED
L37            0 S L36
L38            3 S L36 FULL

     FILE 'HCAPLUS' ENTERED AT 21:06:22 ON 14 MAR 2004
L39            1 S L38
L40            4 S L31 AND YU, K?/AU
L41            9 S L31 NOT L40

=> d 135 and yu, k?/au
'K?' MUST END IN '/Q', '/A', '/L', '/S' OR '/B'
The saved name for a query (or structure or screen set) must end with
'/Q'.  The saved name for an answer set must end with '/A'.  The saved
name for an L# list must end with '/L'.  SDI request names must end
with '/S'.  To see a list of all saved query, answer set,, and L# list
names for this loginid, enter "DISPLAY SAVED" at an arrow
prompt (=>).  Enter "DISPLAY SAVED/S" to see a list of SDI request
names.  Enter "DISPLAY SAVED/B" to see a list of BATCH search
requests.

=> s 135 and yu, k?/au
          2553 YU, K?/AU
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L42 1 L35 AND YU, K?/AU

=> d l42, ibib abs fhitstr, 1

L42 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2002:556140 HCAPLUS
DOCUMENT NUMBER: 137:125159
TITLE: Preparation and antiviral activity of heterocyclic substituted 2-methylbenzimidazole antiviral agents
INVENTOR(S): **Yu, Kuo-Long**; Civiello, Rita L.; Combrink, Keith D.; Gulgeze, Hatice Belgin; Sin, Ny; Wang, Xiangdong; Meanwell, Nicholas; Venables, Brian Lee; Zhang, Yi; Pearce, Bradley C.; Yin, Zhiwei; Thuring, Jan Willem
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 89 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002099208	A1	20020725	US 2001-994012	20011116
WO 2002062290	A2	20020815	WO 2001-US45149	20011120
WO 2002062290	A3	20021121		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1343499	A2	20030917	EP 2001-270116	20011120
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.: US 2000-257139P P 20001220
WO 2001-US45149 W 20011120

OTHER SOURCE(S): MARPAT 137:125159
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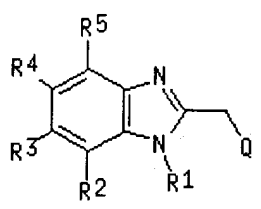

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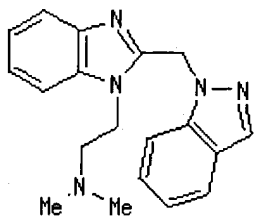


II

AB The title compds. [I; R1 = (CRaRb)nX; Ra, Rb = independently H, C1-6 (un)substituted alkyl; X = H, C1-6 (un)substituted alkyl; n = 1-6; R2, R5 = independently H or halogen; R3, R4 = independently H, halogen, C1-6

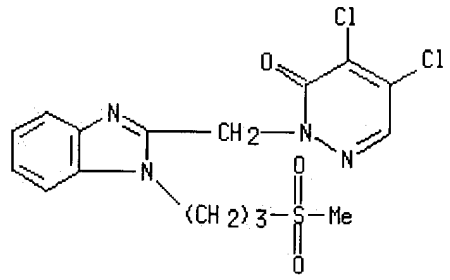
(un)substituted alkyl; Q = heterocyclic group], useful in the treatment of viral infections, more particularly, for the treatment of respiratory syncytial virus infection, were prepd. E.g., a four-step synthesis of II, starting with 2-(chloromethyl)benzimidazole, was given. The antiviral activity of these compds. against respiratory syncytial virus (RSV) was detd. in HEp-2 (ATCC CCL 23) cells. The title compds. I, disclosed herein, show antiviral activity with EC50s between 50 μM and 0.001 μM.

IT **443987-55-1P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. and use of heterocyclic substituted 2-methyl-benzimidazole antiviral agents)

RN 443987-55-1 HCAPLUS

CN 3(2H)-Pyridazinone, 4,5-dichloro-2-[[1-[3-(methylsulfonyl)propyl]-1H-benzimidazol-2-yl]methyl]- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 20:35:55 ON 14 MAR 2004)

FILE 'REGISTRY' ENTERED AT 20:36:00 ON 14 MAR 2004

L1		STRUCTURE UPLOADED
L2	0	S L1
L3	0	S L1 FULL
L4		STRUCTURE UPLOADED
L5	0	S L4
L6	0	S L4 FULL
L7		STRUCTURE UPLOADED
L8	0	S L7
L9	0	S L7 FULL
L10		STRUCTURE UPLOADED
L11	50	S L10
L12		STRUCTURE UPLOADED
L13	50	S L12
L14	2143	S L12 FULL

FILE 'HCAPLUS' ENTERED AT 20:48:14 ON 14 MAR 2004

L15	259	S L14

FILE 'REGISTRY' ENTERED AT 20:48:25 ON 14 MAR 2004

L16		STRUCTURE UPLOADED
L17	50	S L16
L18	1605	S L16 FULL

FILE 'HCAPLUS' ENTERED AT 20:52:42 ON 14 MAR 2004

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L19          210 S L18
L20          183 S L19 AND PD < JANUARY 2001
L21              STRUCTURE UPLOADED
                 S L21

     FILE 'REGISTRY' ENTERED AT 20:56:20 ON 14 MAR 2004
L22            4 S L21

     FILE 'HCAPLUS' ENTERED AT 20:56:21 ON 14 MAR 2004
L23            3 S L22

     FILE 'REGISTRY' ENTERED AT 20:56:27 ON 14 MAR 2004
L24              STRUCTURE UPLOADED
L25            4 S L24
L26           98 S L24 FULL

     FILE 'HCAPLUS' ENTERED AT 20:56:54 ON 14 MAR 2004
L27           13 S L26

     FILE 'REGISTRY' ENTERED AT 20:57:08 ON 14 MAR 2004
L28              STRUCTURE UPLOADED
L29            4 S L28
L30           98 S L29 FULL

     FILE 'HCAPLUS' ENTERED AT 20:59:15 ON 14 MAR 2004
L31           13 S L30

     FILE 'REGISTRY' ENTERED AT 20:59:25 ON 14 MAR 2004
L32              STRUCTURE UPLOADED
L33            0 S L32
L34            7 S L32 FULL

     FILE 'HCAPLUS' ENTERED AT 21:03:33 ON 14 MAR 2004
L35            4 S L34

     FILE 'REGISTRY' ENTERED AT 21:03:40 ON 14 MAR 2004
L36              STRUCTURE UPLOADED
L37            0 S L36
L38            3 S L36 FULL

     FILE 'HCAPLUS' ENTERED AT 21:06:22 ON 14 MAR 2004
L39            1 S L38
L40            4 S L31 AND YU, K?/AU
L41            9 S L31 NOT L40
L42            1 S L35 AND YU, K?/AU

=> s 135 not 142
L43            3 L35 NOT L42

=> d 143, ibib abs fhitstr, 1-3

L43  ANSWER 1 OF 3  HCAPLUS  COPYRIGHT 2004 ACS on STN
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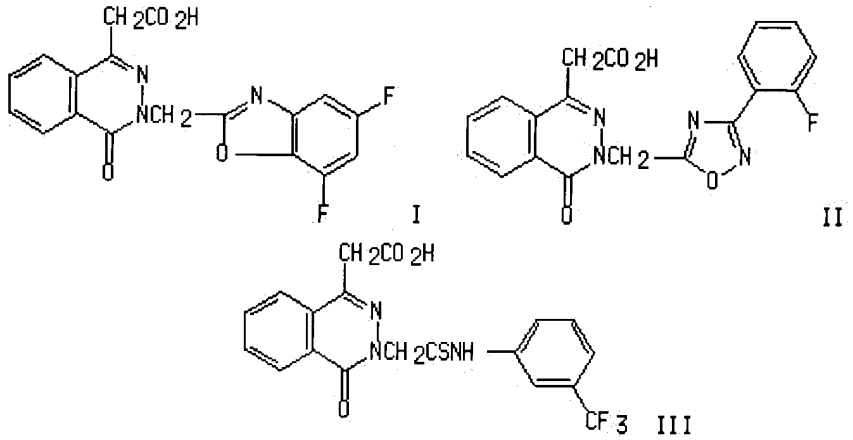
Full Text | Citing References

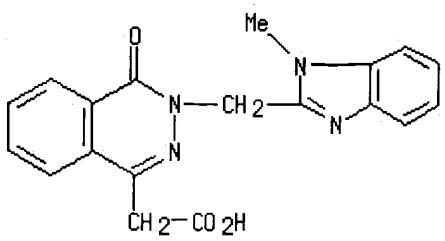
```
ACCESSION NUMBER:         1992:83619  HCAPLUS
DOCUMENT NUMBER:          116:83619
TITLE:                    Potent, orally active aldose reductase inhibitors
                          related to zopolrestat:  surrogates for benzothiazole
                          side chain
AUTHOR(S):                Mylari, Banavara L.; Beyer, Thomas A.; Scott, Pamela
```

J.; Aldinger, Charles E.; Dee, Michael F.; Siegel, Todd W.; Zembrowski, William J.
CORPORATE SOURCE: Cent. Res. Div., Pfizer Inc., Groton, CT, 06340, USA
SOURCE: Journal of Medicinal Chemistry (1992), 35(3), 457-65
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB A broad structure-activity program was undertaken in search of effective surrogates for the key benzothiazole side chain of the potent aldose reductase inhibitor, zopolrestat. A structure-driven approach was pursued, which spanned exploration of three areas: (1) 5/6 fused heterocycles, such as benzoxazole, benzothiophene, benzofuran, and imidazopyridine; (2) 5-membered heterocycles, including oxadiazole, oxazole, thiazole, and thiadiazole, with pendant aryl groups, and (3) thioanilide as a formal equiv. of benzothiazole. Several benzoxazole- and 1,2,4-oxadiazole-derived analogs were found to be potent inhibitors of aldose reductase from human placenta and were orally active in preventing sorbitol accumulation in rat sciatic nerve, in an acute test of diabetic complications. Phthalazineacetic acid I was the best of the benzoxazole series ([C50 = 3.2 x 10-9M); it suppressed accumulation of sorbitol in rat sciatic nerve by 78% at an oral dose of 10 mg/kg. Oxadiazolyl deriv. II with IC50 < 1.0 x 10-8M, caused a 69% redn. in sorbitol accumulation in rat sciatic nerve at an oral dose of 25 mg/kg. The thioanilide side chain features in III proved to be an effective surrogate for benzothiazole. III was highly potent in vitro (IC50 = 5.2 x 10-8M) but did not show oral activity when tested at 100 mg/kg. Addnl. structure-activity relationships encompassing a variety of heterocyclic side chains are discussed.

IT **110703-66-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 110703-66-7 HCAPLUS
CN 1-Phthalazineacetic acid, 3,4-dihydro-3-[(1-methyl-1H-benzimidazol-2-yl)methyl]-4-oxo- (9CI) (CA INDEX NAME)



L43 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

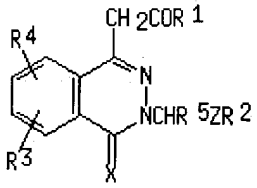
Full Text | Citing References

ACCESSION NUMBER: 1991:81862 HCAPLUS
DOCUMENT NUMBER: 114:81862
TITLE: Preparation of heterocyclic oxophthalazinylacetic acids as aldose reductase inhibitors
INVENTOR(S): Larson, Eric R.; Mylari, Banavara L.
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: U.S., 21 pp. Cont.-in-part of U.S. Ser. No. 136,179.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4939140	A	19900703	US 1988-263577	19881027
CA 1299178	A1	19920421	CA 1986-520609	19861016
DD 254001	A5	19880210	DD 1986-296012	19861106
ZA 8608450	A	19880629	ZA 1986-8450	19861106

PRIORITY APPLN. INFO.: US 1985-796039 19851107
US 1986-916127 19861007
US 1987-136179 19871221

OTHER SOURCE(S): MARPAT 114:81862
GI

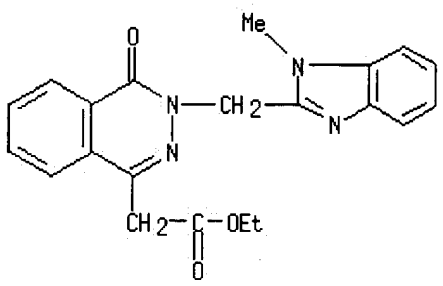


I

AB The title compds. I [X = O, S; Z = covalent bond, O, S, NH, CH2, or CHR5Z = vinylene; R1 = OH, prodrug group; R2 = (substituted) (benzo-fused) 5- or 6-membered heterocyclyl, (substituted) imidazolopyridyl, triazolopyridyl, etc.; R3, R4 = H, F, Cl, Br, CF3, alkyl, alkoxy, etc.; or R3R4 = alkylenedioxy; R5 = H, Me, CF3] were prepd. I are useful as aldose reductase inhibitors (no data). To a mixt. of Et 4-oxo-(3H)-phthalazin-1-ylacetate and NaH in DMF was added 2-(bromomethyl)quinoline. The resulting soln. was stirred at room temp. for 30 min to give a product, which was sapond. to give, after workup, I [X = O, R1 = OH, R3 = R4 = H, CHR5ZR2 = (quinolin-2-yl)methyl].

IT **110703-84-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of aldose reductase inhibitor)

RN 110703-84-9 HCAPLUS
CN 1-Phthalazineacetic acid, 3,4-dihydro-3-[(1-methyl-1H-benzimidazol-2-yl)methyl]-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L43 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1987:576055 HCAPLUS
DOCUMENT NUMBER: 107:176055
TITLE: Preparation of heterocyclic oxophthalazinyl acetic acids derivatives
INVENTOR(S): Mylari, Banavara Lakshmana; Larson, Eric Robert; Zembrowski, William James
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: Eur. Pat. Appl., 41 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 222576	A2	19870520	EP 1986-308545	19861103
EP 222576	A3	19880323		
EP 222576	B1	19920318		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4723010	A	19880202	US 1985-796359	19851107
CA 1299178	A1	19920421	CA 1986-520609	19861016
AT 73801	E	19920415	AT 1986-308545	19861103
IL 80475	A1	19930131	IL 1986-80475	19861103
ES 2032749	T3	19930301	ES 1986-308545	19861103
CA 1293726	A1	19911231	CA 1986-522156	19861104
FI 8604512	A	19870508	FI 1986-4512	19861106
FI 87355	B	19920915		
FI 87355	C	19921228		
DK 8605298	A	19870508	DK 1986-5298	19861106
DK 172010	B1	19970915		
AU 8664858	A1	19870611	AU 1986-64858	19861106
AU 574589	B2	19880707		
CN 86108308	A	19870715	CN 1986-108308	19861106
CN 1009831	B	19901003		
DD 254001	A5	19880210	DD 1986-296012	19861106
ZA 8608450	A	19880629	ZA 1986-8450	19861106
HU 46318	A2	19881028	HU 1986-4621	19861106
HU 206338	B	19921028		
SU 1551246	A3	19900315	SU 1986-4028554	19861106
NO 168303	B	19911028	NO 1986-4425	19861106

NO 168303	C	19920205		
JP 62114988	A2	19870526	JP 1986-265436	19861107
JP 04001747	B4	19920114		
PL 151024	B1	19900731	PL 1986-262266	19861107
US 4748280	A	19880531	US 1987-79869	19870731
CA 1290768	A2	19911015	CA 1990-615750	19900528

PRIORITY APPLN. INFO.:

US 1985-796039	19851107
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EP 1986-308545	19861103
CA 1986-522156	19861104

OTHER SOURCE(S): CASREACT 107:176055

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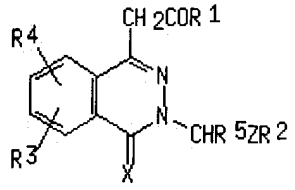


I

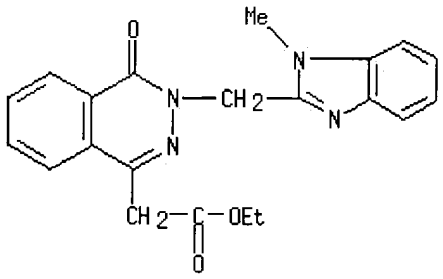
AB The title compds. [I; R1 = OH, 'prodrug' group; R2 = (substituted) (benzo-fused) N-contg. 5- or 6-membered heterocyclyl; R3, R4 = H, F, Cl, Br, CF3, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, NO2; R3R4 = alkanedioxy; R5 = H, Me; X = O, S; Z = bond, O, S, NH, CH2] were prepd. as aldose reductase inhibitors for treatment of diabetes-assocd. disorders (no data). Et 4-oxo-3H-phthalazine-1-ylacetate 11.5 g, NaH, and 5-bromo-2-(bromomethyl)benzothiazole 16.8 g were stirred in DMF for 1 h at room temp. to give 15.6 g I (R1 = OEt, R2 = 5-bromobenzothiazol-2-yl, R3 = R4 = R5 = H, X = Z = O) which (15.0 g) was sapond. with KOH in dioxane to give 7.65 g I (R1 = OH).

IT **110703-84-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and sapon. of)

RN 110703-84-9 HCAPLUS

CN 1-Phthalazineacetic acid, 3,4-dihydro-3-[(1-methyl-1H-benzimidazol-2-yl)methyl]-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 20:36:00 ON 14 MAR 2004

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L3 0 S L1 FULL

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L5            0 S L4
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L7              STRUCTURE UPLOADED
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L10             STRUCTURE UPLOADED
L11          50 S L10
L12             STRUCTURE UPLOADED
L13          50 S L12
L14        2143 S L12 FULL

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L15         259 S L14

     FILE 'REGISTRY' ENTERED AT 20:48:25 ON 14 MAR 2004
L16             STRUCTURE UPLOADED
L17          50 S L16
L18        1605 S L16 FULL

     FILE 'HCAPLUS' ENTERED AT 20:52:42 ON 14 MAR 2004
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L20         183 S L19 AND PD < JANUARY 2001
L21             STRUCTURE UPLOADED
                S L21

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L24             STRUCTURE UPLOADED
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L32             STRUCTURE UPLOADED
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     FILE 'REGISTRY' ENTERED AT 21:03:40 ON 14 MAR 2004
L36             STRUCTURE UPLOADED
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L38           3 S L36 FULL
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L41            9 S L31 NOT L40
L42            1 S L35 AND YU, K?/AU
L43            3 S L35 NOT L42

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L39  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

ACCESSION NUMBER: 2002:556140 HCAPLUS
DOCUMENT NUMBER: 137:125159
TITLE: Preparation and antiviral activity of heterocyclic substituted 2-methylbenzimidazole antiviral agents
INVENTOR(S): Yu, Kuo-Long; Civiello, Rita L.; Combrink, Keith D.; Gulgeze, Hatice Belgin; Sin, Ny; Wang, Xiangdong; Meanwell, Nicholas; Venables, Brian Lee; Zhang, Yi; Pearce, Bradley C.; Yin, Zhiwei; Thuring, Jan Willem
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 89 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002099208	A1	20020725	US 2001-994012	20011116
WO 2002062290	A2	20020815	WO 2001-US45149	20011120
WO 2002062290	A3	20021121		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1343499	A2	20030917	EP 2001-270116	20011120

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRIORITY APPLN. INFO.:	US 2000-257139P	P	20001220
	WO 2001-US45149	W	20011120

OTHER SOURCE(S): MARPAT 137:125159
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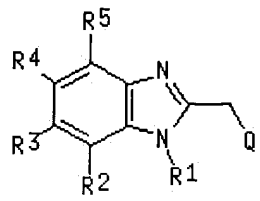

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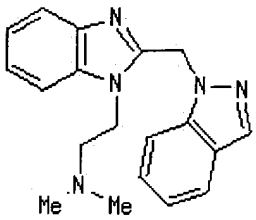


II

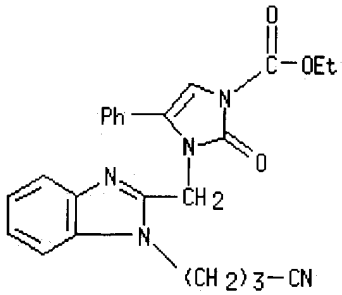
AB The title compds. [I; R1 = (CRaRb)nX; Ra, Rb = independently H, C1-6 (un)substituted alkyl; X = H, C1-6 (un)substituted alkyl; n = 1-6; R2, R5 = independently H or halogen; R3, R4 = independently H, halogen, C1-6 (un)substituted alkyl; Q = heterocyclic group], useful in the treatment of viral infections, more particularly, for the treatment of respiratory syncytial virus infection, were prepd. E.g., a four-step synthesis of II, starting with 2-(chloromethyl)benzimidazole, was given. The antiviral activity of these compds. against respiratory syncytial virus (RSV) was detd. in HEp-2 (ATCC CCL 23) cells. The title compds. I, disclosed herein, show antiviral activity with EC50s between 50 μM and 0.001 μM.

IT **443987-53-9P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. and use of heterocyclic substituted 2-methyl-benzimidazole antiviral agents)

RN 443987-53-9 HCAPLUS

CN 1H-Imidazole-1-carboxylic acid, 3-[[1-(3-cyanopropyl)-1H-benzimidazol-2-yl]methyl]-2,3-dihydro-2-oxo-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



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FULL ESTIMATED COST	99.77	1541.61

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-12.47	-12.47

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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L9           0 S L7 FULL
L10            STRUCTURE UPLOADED
L11         50 S L10
L12            STRUCTURE UPLOADED
L13         50 S L12
L14       2143 S L12 FULL

     FILE 'HCAPLUS' ENTERED AT 20:48:14 ON 14 MAR 2004
L15        259 S L14

     FILE 'REGISTRY' ENTERED AT 20:48:25 ON 14 MAR 2004
L16            STRUCTURE UPLOADED
L17         50 S L16
L18       1605 S L16 FULL

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L19        210 S L18
L20        183 S L19 AND PD < JANUARY 2001
L21            STRUCTURE UPLOADED
               S L21

     FILE 'REGISTRY' ENTERED AT 20:56:20 ON 14 MAR 2004
L22          4 S L21

     FILE 'HCAPLUS' ENTERED AT 20:56:21 ON 14 MAR 2004
L23          3 S L22

     FILE 'REGISTRY' ENTERED AT 20:56:27 ON 14 MAR 2004
L24            STRUCTURE UPLOADED
L25          4 S L24
L26         98 S L24 FULL

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L27         13 S L26
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L29           4 S L28
L30          98 S L29 FULL

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L32             STRUCTURE UPLOADED
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L34           7 S L32 FULL

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     FILE 'REGISTRY' ENTERED AT 21:03:40 ON 14 MAR 2004
L36             STRUCTURE UPLOADED
L37           0 S L36
L38           3 S L36 FULL

     FILE 'HCAPLUS' ENTERED AT 21:06:22 ON 14 MAR 2004
L39           1 S L38
L40           4 S L31 AND YU, K?/AU
L41           9 S L31 NOT L40
L42           1 S L35 AND YU, K?/AU
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L44           1 L26

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L44  ANSWER 1 OF 1  CAOLD  COPYRIGHT 2004 ACS on STN
AN   CA64:6645g  CAOLD
TI   benzotriazolyalkyl benzimidazoles and their dialkylaminoalkyl derivs.
AU   Pagani, Flaminio; Sparatore, F.
IT   5823-54-1   5823-55-2   5823-56-3   5823-57-4   5823-58-5   5823-59-6
     5823-60-9   5823-61-0   5823-62-1   5823-63-2   5823-64-3
     5823-65-4   5823-66-5   5914-83-0   6075-17-8   6075-18-9
     6075-19-0   6075-20-3   6130-50-3   7803-58-9


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FILE 'REGISTRY' ENTERED AT 21:10:29 ON 14 MAR 2004


ANSWER 1  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   5823-63-2  REGISTRY
CN   1H-Benzimidazole-1-ethanamine, 2-(2H-benzotriazol-2-ylmethyl)-N,N-dimethyl-
      (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   2H-Benzotriazole, 2-[[1-[2-(dimethylamino)ethyl]-2-benzimidazolyl]methyl]-
     (7CI, 8CI)
FS   3D CONCORD
MF   C18 H20 N6
LC   STN Files:   BEILSTEIN*, CA, CAOLD, CAPLUS, USPATFULL
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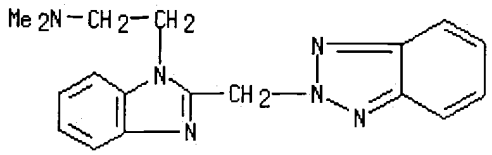
(*File contains numerically searchable property data)



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2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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=> fil reg; d acc 5823-64-3; fil CAOLD

FILE 'REGISTRY' ENTERED AT 21:10:33 ON 14 MAR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 5823-64-3 REGISTRY
CN 2H-Benzotriazole, 2-[[1-[2-(diethylamino)-ethyl]-2-benzimidazolyl]methyl]-, picrate (7CI, 8CI) (CA INDEX NAME)
MF C20 H24 N6 . C6 H3 N3 O7
LC STN Files: CA, CAOLD, CAPLUS

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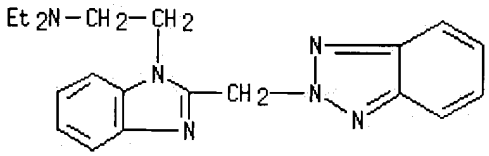
CRN 5914-83-0
CMF C20 H24 N6



CM 2

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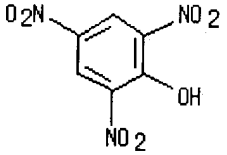
CMF C6 H3 N3 O7



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
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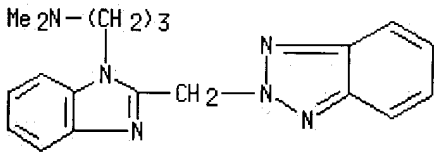
CN 2H-Benzotriazole, 2-[[1-[3-(dimethylamino)propyl]-2-benzimidazolyl]methyl]-, monopicrate (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Benzotriazole, 2-[[1-[3-(dimethylamino)propyl]-2-benzimidazolyl]methyl]-, picrate (7CI)
MF C19 H22 N6 . C6 H3 N3 O7
LC STN Files: CA, CAOLD, CAPLUS

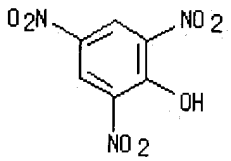
CM 1

CRN 6075-18-9
CMF C19 H22 N6



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



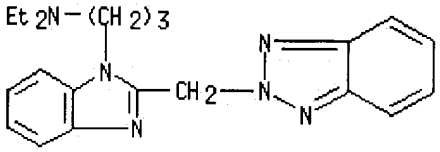
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 21:10:46 ON 14 MAR 2004

=> fil reg; d acc 5823-66-5; fil CAOLD

FILE 'REGISTRY' ENTERED AT 21:10:55 ON 14 MAR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 5823-66-5 REGISTRY
CN 2H-Benzotriazole, 2-[[1-[3-(diethylamino)propyl]-2-benzimidazolyl]methyl]-
(7CI, 8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H26 N6
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

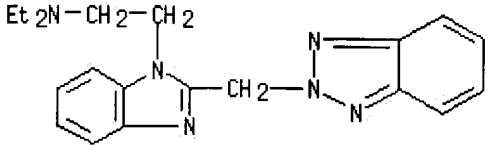
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 21:10:56 ON 14 MAR 2004

=> fil reg; d acc 5914-83-0; fil CAOLD

FILE 'REGISTRY' ENTERED AT 21:11:06 ON 14 MAR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 5914-83-0 REGISTRY
CN 1H-Benzimidazole-1-ethanamine, 2-(2H-benzotriazol-2-ylmethyl)-N,N-diethyl-
(9CI) (CA INDEX NAMES)
OTHER CA INDEX NAMES:
CN 2H-Benzotriazole, 2-[[1-[2-(diethylamino)ethyl]-2-benzimidazolyl]methyl]-
(7CI, 8CI)
FS 3D CONCORD
MF C20 H24 N6
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

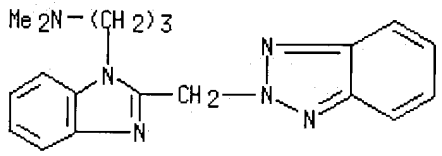
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 21:11:07 ON 14 MAR 2004

=> fil reg; d acc 6075-18-9; fil CAOLD

FILE 'REGISTRY' ENTERED AT 21:11:27 ON 14 MAR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 6075-18-9 REGISTRY
CN 1H-Benzimidazole-1-propanamine, 2-(2H-benzotriazol-2-ylmethyl)-N,N-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Benzotriazole, 2-[[1-[3-(dimethylamino)propyl]-2-benzimidazolyl]methyl]- (7CI, 8CI)
FS 3D CONCORD
MF C19 H22 N6
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 21:11:27 ON 14 MAR 2004

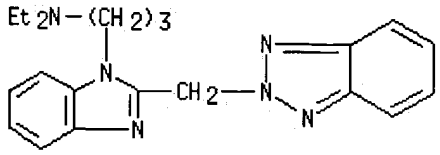
=> fil reg; d acc 6075-19-0; fil CAOLD

FILE 'REGISTRY' ENTERED AT 21:11:33 ON 14 MAR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 6075-19-0 REGISTRY
CN 2H-Benzotriazole, 2-[[1-[3-(diethylamino)propyl]-2-benzimidazolyl]methyl]-, picrate (7CI, 8CI) (CA INDEX NAME)
MF C21 H26 N6 . C6 H3 N3 O7
LC STN Files: CA, CAOLD, CAPLUS

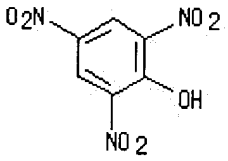
CM 1

CRN 5823-66-5
CMF C21 H26 N6



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



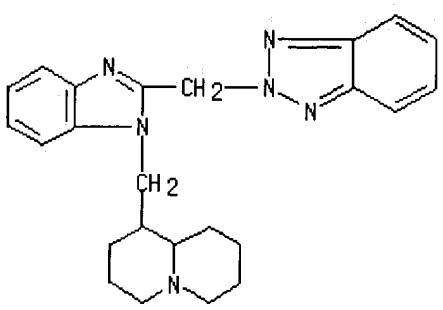
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 21:11:34 ON 14 MAR 2004

=> fil reg; d acc 6075-20-3; fil CAOLD

FILE 'REGISTRY' ENTERED AT 21:11:41 ON 14 MAR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 6075-20-3 REGISTRY
CN Quinolizine, 1-[[2-(2H-benzotriazol-2-ylmethyl)-1-benzimidazolyl]methyl]octahydro- (7CI, 8CI) (CA INDEX NAME)
MF C24 H28 N6
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
FILE 'CAOLD' ENTERED AT 21:11:41 ON 14 MAR 2004

=> d his

     (FILE 'HOME' ENTERED AT 20:35:55 ON 14 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 20:36:00 ON 14 MAR 2004
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           0 S L1 FULL
L4             STRUCTURE UPLOADED
L5           0 S L4
L6           0 S L4 FULL
L7             STRUCTURE UPLOADED
L8           0 S L7
L9           0 S L7 FULL
L10            STRUCTURE UPLOADED
L11         50 S L10
L12            STRUCTURE UPLOADED
L13         50 S L12
L14       2143 S L12 FULL

     FILE 'HCAPLUS' ENTERED AT 20:48:14 ON 14 MAR 2004
L15        259 S L14

     FILE 'REGISTRY' ENTERED AT 20:48:25 ON 14 MAR 2004
L16            STRUCTURE UPLOADED
L17         50 S L16
L18       1605 S L16 FULL

     FILE 'HCAPLUS' ENTERED AT 20:52:42 ON 14 MAR 2004
L19        210 S L18
L20        183 S L19 AND PD < JANUARY 2001
L21            STRUCTURE UPLOADED
               S L21

     FILE 'REGISTRY' ENTERED AT 20:56:20 ON 14 MAR 2004
L22          4 S L21

     FILE 'HCAPLUS' ENTERED AT 20:56:21 ON 14 MAR 2004
L23          3 S L22

     FILE 'REGISTRY' ENTERED AT 20:56:27 ON 14 MAR 2004
L24            STRUCTURE UPLOADED
L25          4 S L24
L26         98 S L24 FULL

     FILE 'HCAPLUS' ENTERED AT 20:56:54 ON 14 MAR 2004
L27         13 S L26

     FILE 'REGISTRY' ENTERED AT 20:57:08 ON 14 MAR 2004
L28            STRUCTURE UPLOADED
L29          4 S L28
L30         98 S L29 FULL

     FILE 'HCAPLUS' ENTERED AT 20:59:15 ON 14 MAR 2004
L31         13 S L30
```

```
     FILE 'REGISTRY' ENTERED AT 20:59:25 ON 14 MAR 2004
L32             STRUCTURE UPLOADED
L33           0 S L32
L34           7 S L32 FULL

     FILE 'HCAPLUS' ENTERED AT 21:03:33 ON 14 MAR 2004
L35           4 S L34

     FILE 'REGISTRY' ENTERED AT 21:03:40 ON 14 MAR 2004
L36             STRUCTURE UPLOADED
L37           0 S L36
L38           3 S L36 FULL

     FILE 'HCAPLUS' ENTERED AT 21:06:22 ON 14 MAR 2004
L39           1 S L38
L40           4 S L31 AND YU, K?/AU
L41           9 S L31 NOT L40
L42           1 S L35 AND YU, K?/AU
L43           3 S L35 NOT L42

     FILE 'CAOLD' ENTERED AT 21:10:08 ON 14 MAR 2004
L44           1 S L26

     FILE 'REGISTRY' ENTERED AT 21:10:29 ON 14 MAR 2004

     FILE 'CAOLD' ENTERED AT 21:10:30 ON 14 MAR 2004

     FILE 'REGISTRY' ENTERED AT 21:10:33 ON 14 MAR 2004

     FILE 'CAOLD' ENTERED AT 21:10:33 ON 14 MAR 2004

     FILE 'REGISTRY' ENTERED AT 21:10:46 ON 14 MAR 2004

     FILE 'CAOLD' ENTERED AT 21:10:46 ON 14 MAR 2004

     FILE 'REGISTRY' ENTERED AT 21:10:55 ON 14 MAR 2004

     FILE 'CAOLD' ENTERED AT 21:10:56 ON 14 MAR 2004

     FILE 'REGISTRY' ENTERED AT 21:11:06 ON 14 MAR 2004

     FILE 'CAOLD' ENTERED AT 21:11:07 ON 14 MAR 2004

     FILE 'REGISTRY' ENTERED AT 21:11:27 ON 14 MAR 2004

     FILE 'CAOLD' ENTERED AT 21:11:27 ON 14 MAR 2004

     FILE 'REGISTRY' ENTERED AT 21:11:33 ON 14 MAR 2004

     FILE 'CAOLD' ENTERED AT 21:11:34 ON 14 MAR 2004

     FILE 'REGISTRY' ENTERED AT 21:11:41 ON 14 MAR 2004

     FILE 'CAOLD' ENTERED AT 21:11:41 ON 14 MAR 2004

=> s 134
L45           0 L34

=> s 138
```

```
L46             0 L38

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.42    1563.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00     -12.47

STN INTERNATIONAL LOGOFF AT 21:12:28 ON 14 MAR 2004
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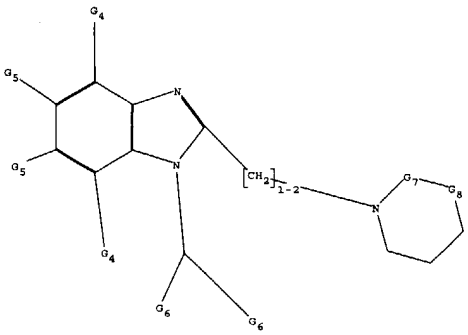
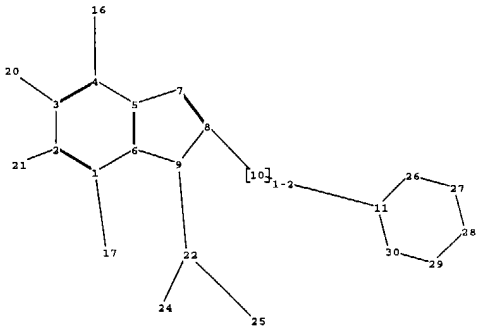




chain nodes :
10 16 17 20 21 22 24 25
ring nodes :
1 2 3 4 5 6 7 8 9 11 26 27 28 29 30
chain bonds :
1-17 2-21 3-20 4-16 8-10 9-22 10-11 22-25 22-24
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-26 11-30 26-27 27-28 28-29 29-30
exact/norm bonds :
1-17 2-21 3-20 4-16 5-7 6-9 7-8 8-9 8-10 9-22 10-11 11-26 11-30 22-25 22-24
26-27 27-28 28-29 29-30
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G4:X,H

G5:X,Ak,H

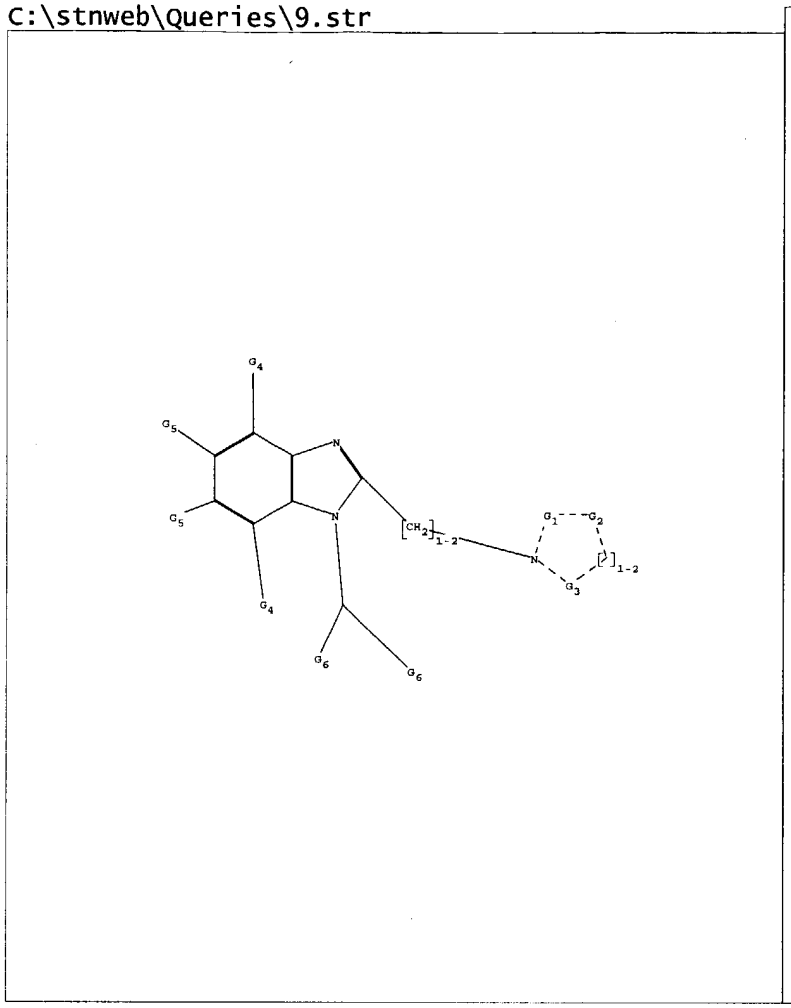
G6:Ak,H

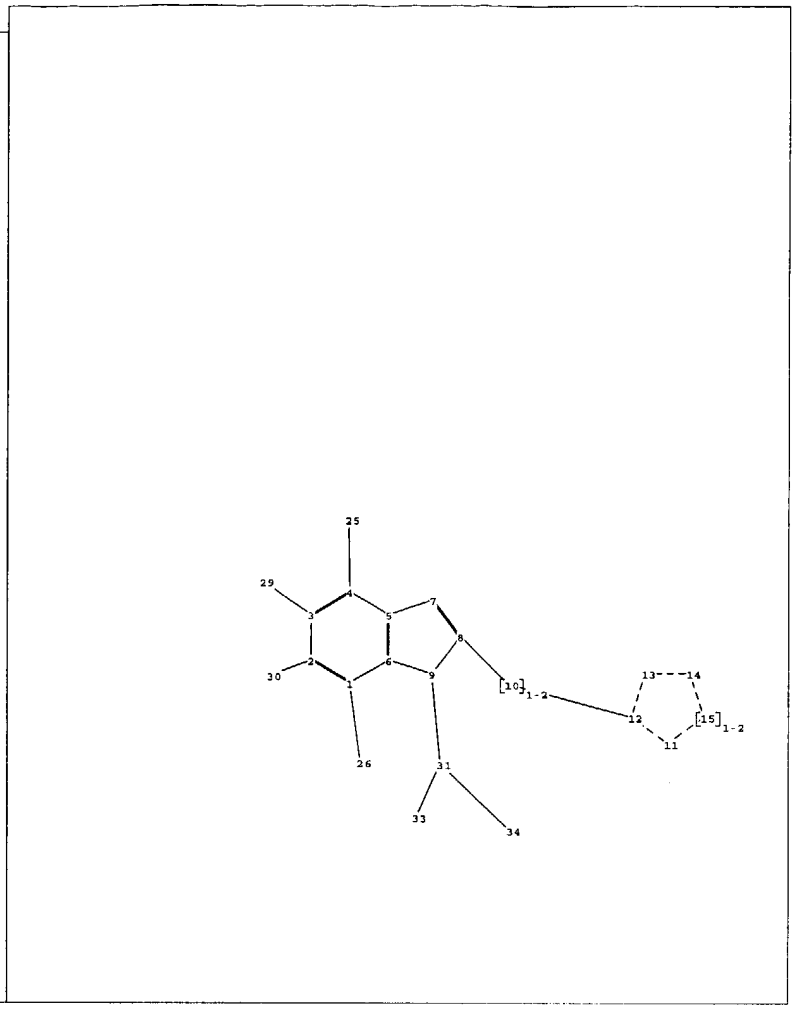
G7:C,S

G8:C,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom
16:CLASS 17:CLASS 20:CLASS 21:CLASS 22:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom
28:Atom 29:Atom 30:Atom

C:\stnweb\Queries\9.str





chain nodes :
10 25 26 29 30 31 33 34
ring nodes :
1 2 3 4 5 6 7 8 9 11 12 13 14 15
chain bonds :
1-26 2-30 3-29 4-25 8-10 9-31 10-12 31-34 31-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-12 11-15 12-13 13-14 14-15
exact/norm bonds :
1-26 2-30 3-29 4-25 5-7 6-9 7-8 8-9 8-10 9-31 10-12 11-12 11-15 12-13 13-14
14-15 31-34 31-33
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:C,S,N

G2:C,O,S,N

G3:C,N

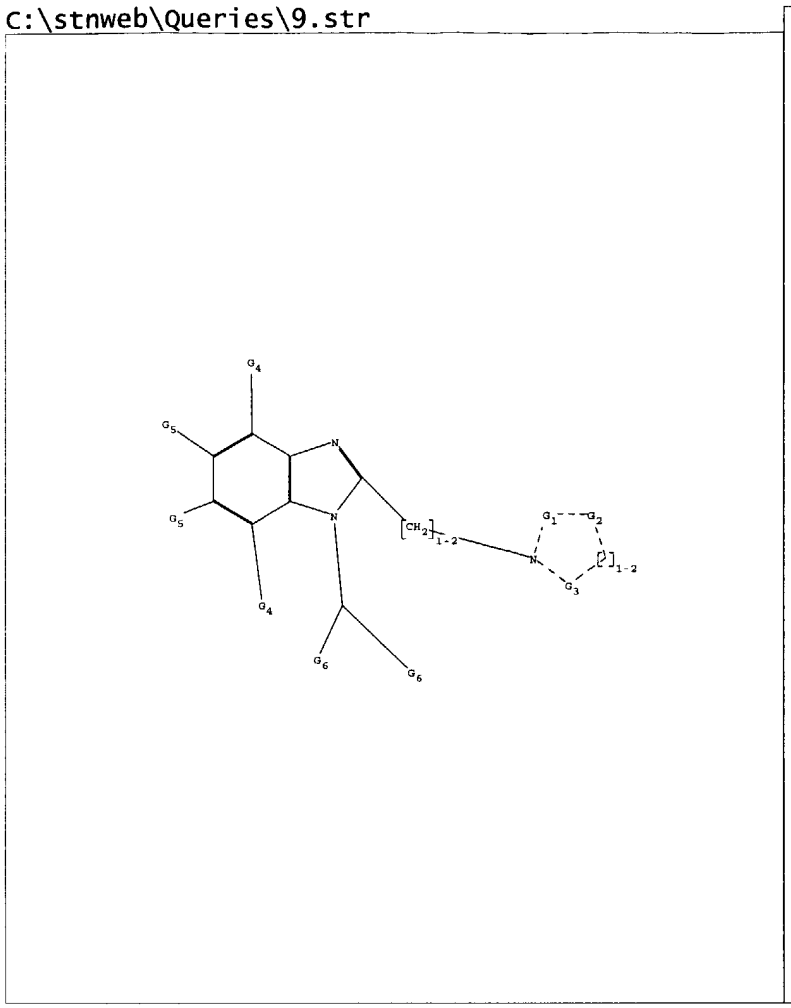
G4:X,H

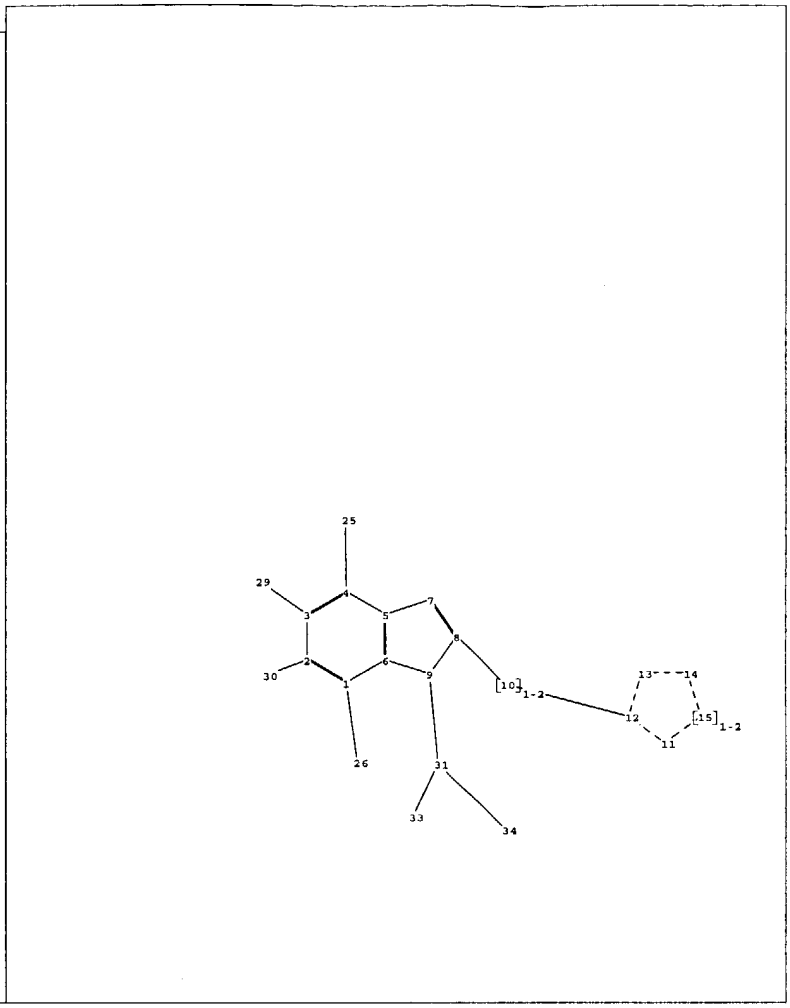
G5:X,Ak,H

G6:Ak,H

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 25:CLASS 26:CLASS 29:CLASS 30:CLASS 31:CLASS
33:CLASS 34:CLASS

C:\stnweb\Queries\9.str





chain nodes :
10 25 26 29 30 31 33 34
ring nodes :
1 2 3 4 5 6 7 8 9 11 12 13 14 15
chain bonds :
1-26 2-30 3-29 4-25 8-10 9-31 10-12 31-34 31-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-12 11-15 12-13 13-14 14-15
exact/norm bonds :
1-26 2-30 3-29 4-25 5-7 6-9 7-8 8-9 8-10 9-31 10-12 11-12 11-15 12-13 13-14
14-15 31-34 31-33
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:C,S,N

G2:C,O,S,N

G3:C,N

G4:X,H

G5:X,Ak,H

G6:Ak,H

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 25:CLASS 26:CLASS 29:CLASS 30:CLASS 31:CLASS
33:CLASS 34:CLASS

```
* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1            Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2            "Ask CAS" for self-help around the clock
 NEWS  3  SEP 09    CA/CAplus records now contain indexing from 1907 to the
                    present
 NEWS  4  DEC 08    INPADOC: Legal Status data reloaded
 NEWS  5  SEP 29    DISSABS now available on STN
 NEWS  6  OCT 10    PCTFULL: Two new display fields added
 NEWS  7  OCT 21    BIOSIS file reloaded and enhanced
 NEWS  8  OCT 28    BIOSIS file segment of TOXCENTER reloaded and enhanced
 NEWS  9  NOV 24    MSDS-CCOHS file reloaded
 NEWS 10  DEC 08    CABA reloaded with left truncation
 NEWS 11  DEC 08    IMS file names changed
 NEWS 12  DEC 09    Experimental property data collected by CAS now available
                    in REGISTRY
 NEWS 13  DEC 09    STN Entry Date available for display in REGISTRY and CA/CAplus
 NEWS 14  DEC 17    DGENE: Two new display fields added
 NEWS 15  DEC 18    BIOTECHNO no longer updated
 NEWS 16  DEC 19    CROPU no longer updated; subscriber discount no longer
                    available
 NEWS 17  DEC 22    Additional INPI reactions and pre-1907 documents added to CAS
                    databases
 NEWS 18  DEC 22    IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
 NEWS 19  DEC 22    ABI-INFORM now available on STN
 NEWS 20  JAN 27    Source of Registration (SR) information in REGISTRY updated
                    and searchable
 NEWS 21  JAN 27    A new search aid, the Company Name Thesaurus, available in
                    CA/CAplus
 NEWS 22  FEB 05    German (DE) application and patent publication number format
                    changes
 NEWS 23  MAR 03    MEDLINE and LMEDLINE reloaded
 NEWS 24  MAR 03    MEDLINE file segment of TOXCENTER reloaded
 NEWS 25  MAR 03    FRANCEPAT now available on STN
 NEWS 26  MAR 29    Pharmaceutical Substances (PS) now available on STN
 NEWS 27  MAR 29    WPIFV now available on STN
 NEWS 28  MAR 29    No connect hour charges in WPIFV until May 1, 2004
 NEWS 29  MAR 29    New monthly current-awareness alert (SDI) frequency in RAPRA

 NEWS EXPRESS  MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

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  result in loss of user privileges and other penalties.

  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:16:55 ON 31 MAR 2004
```
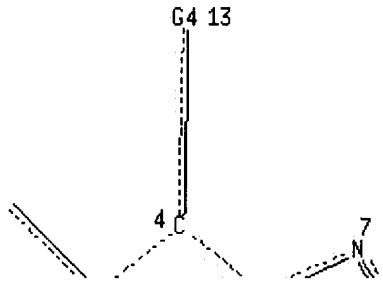
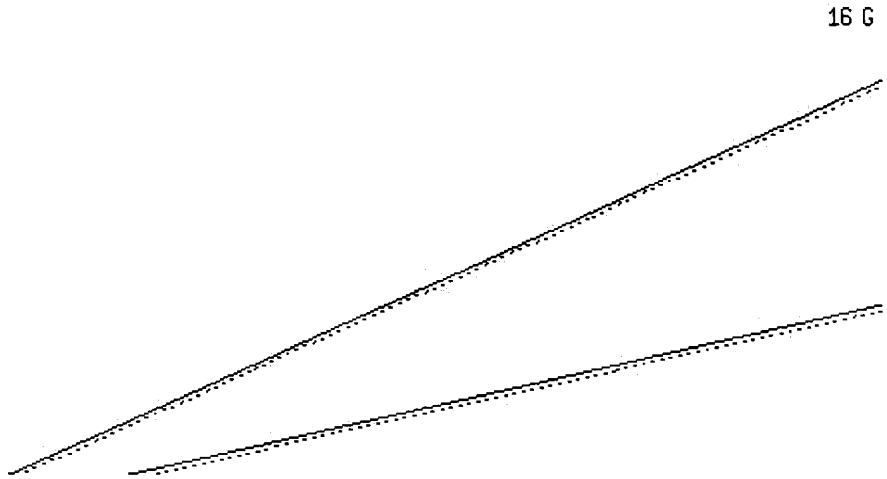

```
=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'REGISTRY' ENTERED AT 14:17:09 ON 31 MAR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   30 MAR 2004  HIGHEST RN 669048-54-8
DICTIONARY FILE UPDATES:  30 MAR 2004  HIGHEST RN 669048-54-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1                STR
 C 34 S 35 N 36


 C 32 S 33


 Ak 30H 31


 X 27 Ak 28H 29


 X 25 H 26
```

15 G5

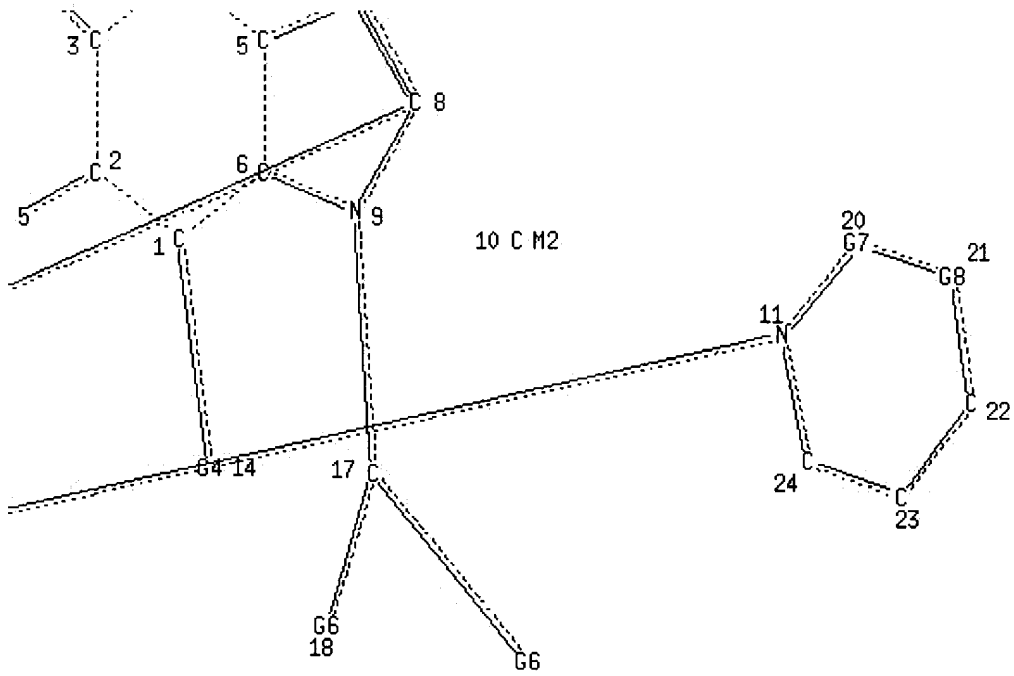
Page 1-A



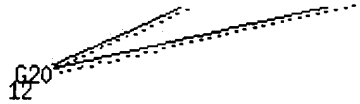
Page 1-B



Page 2-A



Page 2-B



Page 3-A

19

Page 3-B

```
VAR G4=25/26
VAR G5=27/28/29
VAR G6=30/31
VAR G7=32/33
VAR G8=34/35/36
REP G20=(1-2) 10-8 10-11
NODE ATTRIBUTES:
HCOUNT  IS M2     AT  10
NSPEC   IS R      AT   1
NSPEC   IS R      AT   2
NSPEC   IS R      AT   3
NSPEC   IS R      AT   4
NSPEC   IS R      AT   5
NSPEC   IS R      AT   6
NSPEC   IS R      AT   7
NSPEC   IS R      AT   8
NSPEC   IS R      AT   9
NSPEC   IS C      AT  10
NSPEC   IS R      AT  11
NSPEC   IS C      AT  12
NSPEC   IS C      AT  13
NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
NSPEC   IS C      AT  16
NSPEC   IS C      AT  17
NSPEC   IS C      AT  18
NSPEC   IS C      AT  19
NSPEC   IS R      AT  20
NSPEC   IS R      AT  21
NSPEC   IS R      AT  22
NSPEC   IS R      AT  23
NSPEC   IS R      AT  24
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  10 17 25 26 27 28 29 30 31
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   8
NUMBER OF NODES IS  36

STEREO ATTRIBUTES: NONE


=> s l1
SAMPLE SEARCH INITIATED 14:18:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    173 TO ITERATE

100.0% PROCESSED     173 ITERATIONS                          5 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         2671 TO     4249
PROJECTED ANSWERS:               5 TO      234

L2             5 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
```